

Defense, Basic, and Industrial
Research at the
Los Alamos
Neutron Science Center

Proceedings of the Workshop held at
J. Robert Oppenheimer Study Center
Los Alamos National Laboratory
February 12-15, 1995

RECEIVED
NOV 20 1995
OSTI



Edited by Amy Longshore, Group CIC-1

Compiled by Kathy Salgado, LANSCE/ER, and Amy Longshore, Group CIC-1

Cover design by Gail Flower, Group CIC-1

*This work was supported by the U.S. Department of Energy,
Office of Defense Programs and Office of Energy Research.*

An Affirmative Action/Equal Opportunity Employer

This report was prepared as an account of work sponsored by an agency of the United States Government. Neither The Regents of the University of California, the United States Government nor any agency thereof, nor any of their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise, does not necessarily constitute or imply its endorsement, recommendation, or favoring by The Regents of the University of California, the United States Government, or any agency thereof. The views and opinions of authors expressed herein do not necessarily state or reflect those of The Regents of the University of California, the United States Government, or any agency thereof.

*Defense, Basic, and Industrial
Research at the
Los Alamos
Neutron Science Center*

*Proceedings of the Workshop held at
J. Robert Oppenheimer Study Center
Los Alamos National Laboratory
February 12-15, 1995*

DISCLAIMER

Portions of this document may be illegible in electronic image products. Images are produced from the best available original document.

Contents

Abstract.....	1
Introduction	3
PLENARY SESSION	5
Science Policy in Changing Times.....	7
<i>M. R. C. Greenwood, Associate Director, Office of Science and Technology Policy</i>	
Plans for Future Neutron Facilities within the DOE Office of Energy Research.....	12
<i>I. Thomas, Acting Associate Director, Basic Energy Sciences, Office of Energy Research, DOE</i>	
Los Alamos National Laboratory Strategic Directions.....	17
<i>S. Hecker, Director, Los Alamos National Laboratory</i>	
Science-Based Stockpile Stewardship at Los Alamos National Laboratory.....	26
<i>J. Immele, Director, Nuclear Weapons Technology Programs, Los Alamos National Laboratory</i>	
Science-Based Stockpile Stewardship at LANSCE.....	28
<i>J. Browne, Director, LANSCE and Energy Research Programs, Los Alamos National Laboratory</i>	
Why Does Livermore Need LANSCE?	34
<i>R. Fortner, Associate Director, Physics and Space Technology, Lawrence Livermore National Laboratory</i>	
Lab Interdependencies and the Advanced Design and Production Technologies (ADaPT) Initiative.....	37
<i>D. Hayes, Director, Defense Programs Capabilities, Sandia National Laboratories</i>	
TECHNICAL SESSIONS	41
Neutrons for Technology and Science	43
<i>G. Aepli, AT&T Bell Laboratories</i>	
Nuclear Reaction Modeling, Verification Experiments, and Applications.....	56
<i>F. S. Dietrich, Lawrence Livermore National Laboratory</i>	
BREAKOUT SESSIONS	59
Materials Science and Engineering	61
<i>Summary by T. M. Holden, AECL Chalk River Laboratories</i>	
Soft Condensed Matter: Polymers, Complex Fluids, and Biomaterials.....	65
<i>Summary by D. Schaefer, Sandia National Laboratories</i>	
Fundamental Neutron Physics at LANSCE.....	69
<i>Summary by G. Greene, National Institute of Standards and Technology</i>	
Applied Nuclear Physics in Support of SBSS	75
<i>Summary by D. Strottman, Los Alamos National Laboratory</i>	

Condensed Matter Physics and Chemistry	80
<i>Summary by W. J. Nellis, Lawrence Livermore National Laboratory</i>	
The Use of Neutron Scattering in Nuclear Weapons Research	87
<i>Summary by R. J. Juzaitis, Director, Applied Theoretical Physics Division, Los Alamos National Laboratory</i>	
APPENDICES	95
Appendix A: Program	97
Appendix B: Participants	101
Appendix C: Abstracts from the Materials Science and Engineering Breakout Session	106
Computer Simulation of Radiation Effects in Materials	107
Characterization of Explosive Compacts	108
Neutron Resonance Radiography Applied to Explosives Problems	111
Characterization of Stockpile Materials at LANSCE	114
Appendix D: Abstracts from the Applied Nuclear Physics Breakout Session.....	115
Experimental Measurements Supporting the Advanced Fission Model	116
Advanced Post-Scission Fission Model.....	117
Reaction Theory Calculations to 200 MeV for Applications*	118
Appendix E: Abstracts from the Condensed Matter Physics and Chemistry Breakout Session.....	120
Fine-Scale Texture in Complex Electronic Materials	121
Direct Observation of Short-Range Order in Complex Materials	122
Resolving Local Structures on Different Time-Scales Using Neutron Powder Diffraction	123
DuPont's Use of Neutron Facilities	124
Advanced Materials Research Using a Pulsed-Spallation Neutron Source.....	127
Goals for Science-Based Stockpile Stewardship at LANSCE.....	129
Pulsed Neutron Measurements of Excitations in a Quasi-1-D Antiferromagnet	130
Glasses and Crystals in Shocked Tuff, Quartz, and Metals	131
Plutonium Vibrational Spectra at High Pressures and Temperatures	132
The Role of Hydrogen in Earth Processes.....	133
Complementarity of Pulsed Neutrons and High-Energy X-Rays.....	135
Neutron Scattering Investigation of Magnetism in Artificial Metallic Superlattices.....	136
SANS Studies of Magnetic Correlations in Disordered Magnetic Systems.....	137
Structure and Dynamics of Liquids and Amorphous Materials	138
Studying Materials Under Extreme Conditions Using Neutrons	139
Neutron Scattering at High Pressure.....	140

DEFENSE, BASIC, AND INDUSTRIAL RESEARCH AT THE LOS ALAMOS NEUTRON SCIENCE CENTER

*Compiled by
A. Longshore and K. Salgado*

Abstract

The Workshop on Defense, Basic, and Industrial Research at the Los Alamos Neutron Science Center gathered scientists from Department of Energy national laboratories, other federal institutions, universities, and industry to discuss the use of neutrons in science-based stockpile stewardship. The workshop began with presentations by government officials, senior representatives from the three weapons laboratories, and scientific opinion leaders. Workshop participants then met in breakout sessions on the following topics: materials science and engineering; polymers, complex fluids, and biomaterials; fundamental neutron physics; applied nuclear physics; condensed matter physics and chemistry; and nuclear weapons research. They concluded that neutrons can play an essential role in science-based stockpile stewardship and that there is overlap and synergy between defense and other uses of neutrons in basic, applied, and industrial research from which defense and civilian research can benefit. This proceedings is a collection of talks and papers from the plenary, technical, and breakout session presentations.

Introduction

With the end of the cold war and a moratorium on underground testing of nuclear weapons, a new paradigm will be needed to assure the safety, security, and reliability of the remaining U.S. nuclear stockpile. Increasingly, this assurance will depend on a detailed scientific understanding of all aspects of weapons physics coupled with an appropriate predictive capability.

To provide future surety, the Department of Energy (DOE), Office of Defense Programs has initiated programs in science-based stockpile stewardship (SBSS), with the goal of developing a strong scientific underpinning for solving problems that arise in the nuclear weapons stockpile. SBSS will also help attract and retain the technical expertise needed at the country's nuclear weapons laboratories. Some aspects of the problems that weapons scientists will study are of wide scientific interest. An attractive feature of many SBSS programs is their potential to benefit both Defense Programs and U.S. industry. These programs are also expected to attract the interest of basic research communities in areas as diverse as materials science and astrophysics.

Los Alamos National Laboratory proposes to make accelerator-based spallation neutron sources a central element of its contribution to science-based stockpile stewardship. Existing neutron sources at the Laboratory are being improved to enable a variety of experiments including neutron scattering investigations of materials, high-energy neutron radiography, and the measurement of nuclear cross sections. Simultaneously, the Laboratory is undertaking a high-priority program to develop the technologies required for the accelerator production of tritium. Studies are under way of high-power spallation sources for research, including a 1-megawatt long-pulse source that could be built cost effectively using the Laboratory's existing

high-power proton linear accelerator. The Laboratory has developed strategies that would enable the transmutation of long-lived nuclear waste and the generation of clean nuclear power using accelerator-based neutron sources.

This volume contains the proceedings of the workshop held at Los Alamos between February 13th and 15th, 1995, at which a more complete vision for the use of neutrons in SBSS was developed by over 200 scientists from the DOE's national laboratories, other federal institutions, universities, and industry. After the first day of plenary presentations by government officials, senior representatives of the three weapons laboratories, and scientific opinion leaders, the workshop broke into groups to explore the overlap and mutual synergy between defense and other uses of neutrons in the areas of basic, applied, and industrial research. At a separate classified session before the workshop, participants from the defense programs laboratories identified known or potential stockpile problems that could be addressed using neutrons. An unclassified summary is included in these proceedings.

Several clear conclusions emerged from this workshop. Perhaps the most important confirmed the essential role that neutrons can play in stockpile stewardship. The synergy and overlap between the interests and needs of the defense, basic, and industrial research communities were also striking. A future in which these communities can work together for mutual benefit is clearly supported by the interest and interactions that this workshop generated among scientists with widely different backgrounds.

Roger Pynn
John Browne
Los Alamos National Laboratory

PLENARY SESSION

*Workshop on Defense, Basic, and Industrial Research
at the Los Alamos Neutron Science Center*

Science Policy in Changing Times

M. R. C. Greenwood, Associate Director,
Office of Science and Technology Policy

Introduction

Like many scientists who were born right after World War II and who have learned a lot about physics, physical sciences, and biology from some of the incredible discoveries that were made in the defense laboratories, I have always been fascinated with Los Alamos. One of the marvelous opportunities that my job in Washington presented was to get to know a good deal more about the physical science world and the Department of Energy (DOE) laboratories, particularly Los Alamos since the Manhattan Project.

History, however controversial it may be in today's world, will certainly show the critical role that Los Alamos National Laboratory played in foreshortening World War II. This role may be difficult to understand in today's contemporary society where so many of our citizens are scientifically illiterate and do not have a real appreciation for what it is that physical sciences, nuclear sciences, and the atomic age brought to this world. I think that time and testimony will show the great breakthroughs that allowed us to look at the world differently at the turn of the century than we did after World War II.

Science Policy Changes Drastically

What I would like to talk about is how dramatically science policy is changing. It is pressured for many reasons. One of which is, with the end of the cold war or perhaps with the change of the cold war (with this audience I am not sure I would venture to say the cold war is over), that our nuclear and our national security challenges have changed. We have several factors that put tremendous pressure on science policy making and on the science budget right now. Certainly one pressure is that the political climate has changed in the national security arena. Many of our citizens and legislators perceive that the national security environment has changed so much that

some of the justification for scientific research and particularly nuclear research has eroded. Many believe we have a lesser need for some of the facilities and operations than we have had in the past. In addition, a populous movement is going on in the country right now that is putting on pressure to decrease the size of government and to put money back in the pockets of taxpayers. Science and technology, which have historically been great drivers for the economic and intellectual future of the country, are not necessarily seen that way by those who are in a position to determine the long-term budgets for science and technology today.

In addition, an increasing skepticism exists among many of our citizens about the value of science and technology. In journals such as the *Chronicles of Higher Education*, more and more articles raise the issue of skepticism—does science do as much for us as it claims or does it do more harm than good? Some of these articles are well written, well reasoned, and convincing, and I think increasingly we are facing political changing times as well. So, between the changing national needs and the pressure to engage in the “anything you can cut, I can cut better” game, I think we are facing some extraordinary challenges.

A Brief History of Science Policy

Let me talk about what many of us would remember as the seminal science policy document of the last century that defined the science policies that have generated the world-class research and development operation that we have in the United States today. Vannevar Bush's, *Science the Endless Frontier*, which he wrote as the science advisor to President Truman at the conclusion of World War II, has served as a guide for United States science policy for the past 50 years. It provided much of the justification for the U.S. to establish the most powerful scientific enterprise in the world. It has provided not only for our na-

tional security, but also in many ways for our general well-being.

Nonetheless, as I mentioned earlier, in the intervening 50 years, enormous changes have taken place both internationally and within our own society. One could argue, for example, that the overall research and development (R&D) budget has been largely influenced by two major drivers; one is the need for national security, and the other is the need for health and well-being. Today there are at least five, which include not only national security and health, but also environmental security, economic security, and personal security (a freedom from violence, a better understanding of the social structures of our society, and some ability to contain what many people individually perceive as chaos and danger in their personal lives).

Because of this demand for science to step up to the plate, not only in national security and health, but in some of these other areas, Dr. Gibbons asked me to emphasize the role of science in the Office of Science and Technology Policy (OSTP). A perception existed that OSTP was very interested in technology policy but that we were not carrying the ball as much as we should in science policy. So we convened a national forum called, "Science in the National Interest." Some of you and many of your colleagues were at that forum.

National Science Forum Convened

We brought together about 300 scientists from around the country and from broadly distributed fields—physical science, chemistry, biology, life sciences, social sciences. We also brought together folks who were in policy making and bench scientists. We worked very hard to bring in some young scientists and a more diverse mixture of scientists than has perhaps been the typical case in past meetings. As a result of the exercise and with extensive input, not just at the forum but from many people who helped us develop it, President Clinton and Vice President Gore released in August a new policy document called, *Science in the National Interest*. It builds on the previous decades of successful stewardship of science. It has deep bipartisan roots. For exam-

ple, the previous administration's President's Council of Science and Technology (PCAST) report is very much a basic part, as is the National Academy's COSEPUP report, and strong elements are in the Carnegie Foundation's recent reports.

Science in the National Interest is primarily different because it speaks of science, science policy, and science and technology's relevance to society in a much more people-oriented way. It talks about the necessity of the American public to understand what the scientific R&D enterprise is about, it talks about the responsibility that scientists have to communicate both the excitement and opportunities that their fields bring, as well as to be honest when there are risks that need to be evaluated. It talks about pulling the science community together rather than fracturing it into disciplinary bases. The document identifies science with the national interest by elaborating its relationship with the strategic goals that were articulated the first months of the Clinton administration.

Strategic Agenda Moves Forward

If you look at the way the science and economic policies of this administration rolled out, albeit stressed by the changing political environment, a set of specific strategic goals were pursued in this administration. One of them was that long-term economic growth creates jobs and protects the environment. Any objective evaluation of the first 2 years of the Clinton administration's impact on the economy and the jobs would show that we have done a fine job with our policies in trying to move this agenda forward.

A second part of this strategic agenda was a government that is more productive and more responsive to the needs of its citizens. This effort is led by the vice president and involves many of you. The bottom line is that the federal government has the smallest number of full-time employees (FTEs) now, at the end of 2 years of the Clinton administration, than it has had since the Kennedy administration. There are a hundred thousand fewer FTEs and many would argue that much of what has been done has effectively increased efficiency and is

moving forward. There is more to do. This group knows much about the proposed saving from economies and efficiencies at DOE. This downsizing movement, which has now affected government, is not fundamentally different from movements that have been prevalent in industry over the past decade.

Finally, an additional goal that was in the first set of the administration's strategic goals was "world leadership in basic science, mathematics, and engineering." This goal is where OSTP development of the document, *Science in the National Interest*, began. *Science in the National Interest* also put forward the particular goals associated with maintaining world leadership in basic science, mathematics, and engineering. These goals are broad, but they can lead to very specific forward movements:

- Maintaining leadership across the frontiers of scientific knowledge
- Enhancing connections between fundamental research and national goals
- Stimulating partnerships that promote investments in fundamental science and engineering and effective use of physical, human, and financial resources
- Producing the finest scientists and engineers for the twenty-first century
- Promoting a national effort to raise the scientific and technological literacy of all Americans

If we do not find a mechanism to improve the national interest in science, there will not be any science in the national interest for the future. Although the last goal is, in many ways, the most difficult challenge for the nation, it may be the one that is most important for ensuring that we invest in science and technology for the future of the nation.

This document was well received by a range of the public and by the scientific community that had previously regarded the Clinton administration as giving new scientific discovery a lesser role than the application of scientific knowledge to industrial productivity. I do not think that was ever the intention.

Science and Technology Budget Difficult to Sustain

Using *Science in the National Interest*, we worked with the National Science and Technology Council's (NSTC's) committees including the Committee on Fundamental Science to address budget priorities. It was an imperfect process—one that we hope to improve next year but nonetheless a useful one. We looked across all the agencies—National Science Foundation (NSF), National Institutes of Health (NIH), DOE, Department of Defense (DoD), Department of Agriculture, and so forth, to see what they were doing in what we defined as fundamental science, and we performed a broad spectrum disciplinary analysis. The analysis clearly pointed out that the deepest difficulties we were having in the 1996 projected budgets were in sustaining the physical science efforts in the mission-oriented agencies. It was clear that DOE, NASA, and DoD's science efforts were under stress. Although NIH and NSF were not getting the double digit increases that they had gotten in other times, at least they were moving in a forward direction.

We are having difficulty with the science and technology budget. The bottom line is that the discretionary budget of the government is under terrific pressure because of the upward spiral of the mandatory outlays plus the interest on debt portions, which are demanding a substantial portion of the federal budget. The attractiveness of deficit reduction plus a middle-class tax break, which both parties are interested in accomplishing over the next decade, really constrains the resources that we have. As a consequence, the overall opportunities for improving a science and technology effort are largely confined to trying to make better use of the funding that we already have as opposed to expecting any substantial influx of funding into the R&D budget.

In the administration's 1996 proposed budget, total R&D remains constant, but basic research has gotten a substantial increase, 3.5%, while development was decreased (Figure 1). This illustrates that the principles we were espousing of trying to improve the science investment, trying to move some funding out of

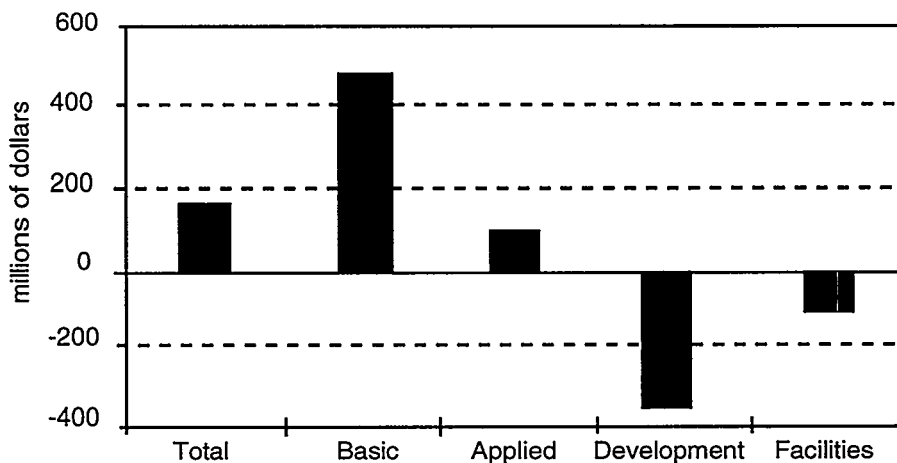


Figure 1. Change in R&D spending from 1995 to 1996.

the development area and into specific science and precompetitive technology efforts as well have been accomplished within the envelope that we were using.

Science Investments Show a Return

An important factor that has contributed to our ability to sustain this investment has been the firm belief among the president's economic advisors that there is a very high rate of social return on federal investments, particularly in fundamental and in precompetitive applications-oriented research with a range of 20% to 400% return. Most economists agree that this is a higher rate of return on investment than other types of investments that are made in the private sector. This fact has helped support the argument that the nation needs to continue to invest in science and technology even if in a tax-cutting mode. Scientists need to encourage the economic scholars in our midst to continue to evaluate the national investment in R&D and get the story out that investment in this area is a good use of government money.

The administration has also believed that supporting basic research at universities or in university-lab or university-industry collaborations is a good use of funding because it not only generates new ideas and potentially patentable ideas and products, but it is also training the next generation of scientists and ensuring that we have a new set of ideas that come into the field over the next 20 years.

The DOE overall budget increased by only 1.7%, and the R&D budget shows about a 7.4% increase. Part of this increase directly reflects why we are here today. We are particularly pleased to move forward an administration and DOE initiative of 100 million dollars for increased use of DOE's state-of-the-art user facilities such as the Los Alamos Neutron Science Center (LANSCE).

Support Comes from All Over

I want to call to your attention this particular facilities initiative for two reasons. One reason is that this initiative is a very good thing and is going to need your support in ensuring that it survives the legislative season. The second reason is that this initiative illustrates the kinds of initiatives which build on existing, underutilized facilities and on existing physical and human resources that might be most successful over the next few years. It is an example of good government. Rather than going ahead and moving with something new, we are trying to make the most of what we have and increase the efficiency. It meets the REGO—reinventing government—criteria.

There are also appreciable additions to the R&D budget from DOE/Defense Programs (DP) including the operation of the linac that will provide the protons for LANSCE. I find this support of the significant research facilities by DP very heartening, and we are delighted with the vision that Vic Reis has brought to his position. Bringing together the

DP and Energy Research scientists in very productive ways for the future is something that I think also meets the criteria for REGO and moving us forward for the 21st century.

The proposed use of spallation neutrons is an exciting technological development that may be the best hope for providing the U.S. research community with a world-class neutron source. The administration proposes postponing, perhaps not doing, the Advance Neutron Source because of the costs, and we are interested in the outcome of the discussions here about the future neutron needs of the country.

The recent Galvin report to the secretary of energy lends much support to the initiatives that are being put forward both specifically in terms of the agency's overall mission and the Los Alamos mission within the agency. OSTP did find a vigorous defense of DOE's mission in high-energy, nuclear, and condensed-matter science heartening and trust that you did as well. One of the sentences that I found particularly gratifying is that the role that DOE plays in sustaining the long-term national interest and the investment in discovery knowledge in fundamental research is a proper role for DOE and one we hope will continue.

Science and Technology Budget is Sound

The administration's fiscal year 96 budget could be defended and in fact was defended in a recent editorial in the *New York Times* as a responsible presidential budget; it will be difficult to hang onto that budget as it goes through the legislative process.

Another effort that was tried, in the spirit of reinventing government, was to make some improvements in the cost of research for universities. In the reform of research activities, research facilities and operations, and research administration, a number of administrative and facility processes were tightened that will save money. The Clinton administration's current policy on that is any saved money ought to be returned to be invested into the science and technology enterprise. This is the solid position taken in the face of an arbitrary cap that would be extremely damaging to many institutions and that has absolutely no theoretical basis in supporting the cost of research.

Changing the National Opinion

In *Science in the National Interest*, we said we must elevate the nation's understanding of the importance of science and technology for the future of our children, our grandchildren, and our economic and national security. Japan, Germany, and other countries with which we compare ourselves are improving the level of their overall federal and private investment in R&D to approximately 3% of their gross domestic product. Admittedly, we are a larger country, and the overall investment we make in R&D is still substantially larger than what our competitors invest. Nonetheless, economists argue that the economic success of a country is tied to its investment in R&D. We have to move the country forward in ways that will allow us to develop the resources necessary to do the important work that I know all of you and your colleagues around the country can do.

Plans for Future Neutron Facilities within the DOE Office of Energy Research

*I. Thomas, Acting Associate Director,
Basic Energy Sciences, Office of Energy Research, DOE*

Introduction

M.R.C. Greenwood brought out some things about the importance of making sure that the public, who funds our work, knows that there is value to it. Currently, the Basic Energy Sciences (BES) advisory committee has a panel that is doing just that for BES research. I insisted that this panel not be the same folks. It is chaired by an economist and it has several nontechnical members on it. I wanted them to have some, you might say, people off the street on it. I have some confidence that often when you bring things to the people, you get good decisions.

A case before the courts in Boston had to do with some highly pathogenic research. As I recall, the citizens on that jury were a mailman, a mechanic, and so forth, and they were having to make decisions on some very technical issues. They came out with a set of guidelines that were very good. Even though they were not technical at all in the field, when presented with the facts, they said here is what we think you should do. The court recognized the value of this input. So sometimes bringing in the outside community, which we tend to be afraid of, is not a bad idea as long as they are reasonable. There are always fringes out there that you have to worry about.

I have also started economic studies in BES to find out what is the impact of the research that we do and on performance measures. Congress said we had to do it; however, I decided to find out which performance measures make sense.

A Brief History of User Facilities

I thought I would start out with some good news. Why our facilities are important, and why the initiative was important? For one thing, we have a lot of facilities within BES because we are always pushing the envelope.

This whole complex was born out of the Manhattan Project, which essentially was pushing the envelope on everything—chemistry, physics, and so on. For example, we have electron microscopy centers. If you go back in history, we became interested in electron microscopy because we found out that you could examine radiation damage using electron microscopes. You could look at the damage that was being caused in materials. Then you start pushing the characterization techniques. I guess the isotopes were a very important part of trying to understand the rest of the periodic chart. The isotopes were first being created by this predecessor agency of ours. This whole complex of facilities grew out of this need.

Originally these facilities were not user facilities. They were built for the purposes of the Atomic Energy Commission, particularly the research reactors. Scientists across the country wanted to do some research at them, so they were opened in a collaborative mode. If you were a scientist somewhere and wanted to do some research at the High-Flux Research Reactor (HFBR), you called up the scientist that you knew at the laboratory and started doing research. I remember in 1974 I submitted a proposal to the National Science Foundation (NSF) to establish a formal user facility in crystallography at the High-Flux Isotope Reactor (HFIR). We were doing crystallography, but we were only using the instrument 30% of the time. I thought why not use it a full 100% of the time. NSF was not comfortable with that idea and neither was the then equivalent to the Department of Energy (DOE).

Out of these efforts comes the recognition that these important facilities needed to be opened to everybody. We finally built what I consider the first from the ground-up user facility, which was the National Synchrotron Light Source (NSLS). I am talking about Basic Energy Sciences facilities not the high-energy facilities, which are very different. From our

standpoint, the NSLS was the first ground-up user facility. After that, we "saw the light" and opened other facilities and made them user facilities that have user groups and program advisory committees of the users. In addition, we have smaller facilities, for example, electron microscopes, that do not really have large operating costs but are important to some people. We do research at them and it is not a question of buying electricity or fuel or whatever, so we let users into these facilities. Some of the facilities were then unique, like the atomic resolution microscope at the National Center for Electron Microscopy (NCEM) at Berkeley and the Shared Research Equipment Program (SHaRE), a collection of instruments at Oak Ridge.

Financial Impacts on User Facilities

Many people use these facilities. This is small science done in a single location. The same people that would do x-rays with a rotating anode or any kind of x-ray machine are the same people that would go to the NSLS or the Advanced Light Source (ALS) to do experiments. They are not the large teams that you see in high-energy and nuclear physics. Without the Scientific Facilities Initiative (SFI) we were saturated; we could not provide any more support, time, or anything else. Users come primarily from the material science disci-

plines—condensed-matter physics, metallurgy, ceramics, and so on. In addition, there is a large group of chemists and biologists, and a smaller number of geologists. Users come from across all the physical and natural sciences. The SFI has had a big impact on the BES budget. This budget is going to be very tough to maintain and can be compared to low hanging fruit. Any time there is an increase the easiest thing to do is to not give it. This way you save that money, and you have not hurt anybody.

How does this impact the specific facilities? Table 1 shows the operating dollars for the facilities. Each budget buys the electricity, fuel, and in some cases also provides user support, in the sense of people to help the users. The other part of SFI has to do with instrumentation. Roughly half of the 57 million dollars that is coming into BES through these facilities is going for instrumentation. Another 3 million is going for the supercomputer center. We will be going out with a notice of program interest or some mechanism so we can have a competitive process for selecting those instruments. We are also going to be asking people to amplify the funds. I did not use the word leverage because I never know where the fulcrum point is. We certainly want industries and states involved in helping to amplify these funds for their purposes.

*Table 1. FY 1996 Congressional Budget, Basic Energy Sciences
Operating Expenses - Facility Operations, B/A (Dollars in Thousands)*

<i>Facilities</i>	<i>FY 1994</i>	<i>FY 1995</i>	<i>FY 1996 Cong Request</i>
High-Flux Beam Reactor	\$21,728	\$21,100	\$24,863
National Synchrotron Light Source	23,377	23,491	27,818
Combustion Research Facility	4,171	4,171	4,592
Radiochemical Engineering Development Center	7,469	7,070	7,549
High-Flux Isotope Reactor	25,414	24,248	28,080
Intense Pulsed Neutron Source	6,843	6,800	11,335
Manuel Lujan Jr. Neutron Scattering Center	2,052	0	6,970
Stanford Synchrotron Radiation Laboratory	13,329	13,427	18,398
Advanced Light Source	21,825	21,200	29,915
6-7-GeV Synchrotron Radiation Light Source	52,380	64,900	82,520
Undesignated	0	*1,3041	0
Total Facility Operations	\$178,588	\$187,711	\$242,040

* Funds for major use facilities; this amount reduced at the appropriation level as a share of prior year balance reduction.

One reason we are here is the Los Alamos Neutron Science Center (LANSCE). You notice that LANSCE has zero dollars in fiscal year 1995. LANSCE is a triple-use facility that originally relied on protons from the Clinton P. Anderson Meson Physics Facility (LAMPF), which is funded out of nuclear physics; the proton storage ring, which came out of the weapons program; and our funds out of BES for the Manuel Lujan Jr. Neutron Scattering Center. We built the experiment hall and the other parts were already there. Nuclear physics decided they were through with LAMPF. They are still doing some beautiful experiments there. Nevertheless, nuclear physics is not going to fund it anymore because it is not a priority. We cannot afford to operate it, therefore, we put LANSCE in shutdown mode.

Before we had the stockpile stewardship program, Defense Programs (DP) funding for LANSCE and the Weapons Neutron Research program was declining. The stockpile stewardship program, however, made a profound change. I was in one of the workshops you had for stockpile stewardship. Going into that workshop I think LANSCE and neutron scattering was a very low priority for 80% of the people. As we progressed in the discussions and people started asking, "how are you going to find out what is happening to your materials," the priority kept bubbling up. Finally it was around second. In the past, you could go test weapons, and we did not really know about the alternatives. Now suddenly neutrons become important because weapons cannot be tested. This shift changes the whole picture for us because now somebody else is going to fund the operation of LAMPF, and we can continue supporting what Energy Research (ER) is interested in, which is research in condensed-matter physics and all the other good things we can do with neutrons.

Initiatives within Basic Energy Sciences

Other initiatives in BES include environmental technology partnerships, sustainable development, and a partnership for new generation vehicles. Environmental Technology Partnerships refer to fixing the science-based, tech-

nological problems in the four major industries that account for roughly 80% of the pollution in this country. Sustainable Development refers to doing it right the first time. If you are going to make a material, make it so it can be recycled or it can be disposed of in an environmentally safe manner. Partnership for New Generation Vehicles refers to not buying a new car because once we start this program we are going to get much better cars.

The last initiative is a Spallation Neutron Source, which is the beginning of a conceptual design of a spallation neutron source. That is the good news. By the way, what you are hearing is the gospel according to Thomas. Clearly Martha Krebs and Jim Decker might not totally agree with everything that I am saying.

What does ER want from LANSCE? The same thing that users want—continual, reliable operation. Reliability is the most important thing. We want higher currents. The original three-party agreement that resulted in building the facility—the experiment hall and all that—called for 100 μ A. We have not gotten there yet. There is talk about working together—ER and DP. We have significant commitments at the DP laboratories. Let me point out that the neutron scattering facility here originated with the commitment from nuclear physics and our support for an experiment hall. We support Los Alamos in neutron scattering research and also in a very significant materials program.

At Sandia National Laboratories, we have a Combustion Research Facility, which sounds far away from weapons work but it turns out that more funding at the Combustion Research Facility is from DP than from the Office of Energy Efficiency. This makes sense because weapons have a little bit of everything in them. Many of the explosives are essentially a way of burning things in a slightly more violent way than we like to see in automobiles. It is essentially a laser facility, and we are doing chemical physics. We have a significant materials program at Sandia also. More importantly, Sandia is responsible for the virtual laboratory, the Center for Excellence for Synthesis and Processing, that we have created.

They coordinate the efforts of 13 laboratories in that area. We have a very strong commitment at the weapons laboratories.

We also have a research program at Lawrence Livermore National Laboratory, and it is working with the Berkeley combustion dynamics initiative and at the ALS. The funding we provide for these laboratories is minuscule compared with their total funding, so I always ask the laboratory directors why they are bothering with this funding? Why are you wasting your time dealing with another office? They tell me that the funding we provide is vital to the health of the laboratories. If that is true, I assume that it is important to stockpile stewardship also. We are very much in a partnership with DP. We have a very strong commitment, and in turn we get a lot for our money. We do from all of our laboratories.

On the other side, I think that stockpile stewardship is going to require the kind of facilities that we have—the Advanced Photon Source (APS), ALS, and so on. I would like to see DP looking at these more seriously from the standpoint of what they can contribute to science-based stockpile stewardship. A requirement for all of our facilities has always been that classified research would be allowed.

I have given you the good news. The bad news is that the Advanced Neutron Source will not be continued in 1996—it has been postponed, deferred. Three billion dollars is just too much in this climate. The neutron scattering community has a lot invested in the facility. Many people are disappointed that the nation is not going forward with it. It was born with community involvement from the start. I was involved with it from the start also, and I am disappointed. It causes a major change in ER's plan for materials research facilities.

The Vision for Basic Energy Sciences

I want to talk about vision and if we know where we are going. Let me go back to how these facilities got started. The community in the late 70s began to make clear that neutron sources could be improved significantly because of the developments at the Institut Laue-Langevin. There were several national

research council reports. In the early 80s, we had the Eisenberger-Knotek report on the need for synchrotrons going beyond NSLS because of the arrival of insertion devices, undulators, wigglers, and so on, which changed the way one could use these machines. Finally, these thoughts culminated in the 1984 long-range plan in the Division for Material Sciences, which established the vision for these facilities.

We said we needed a ultraviolet light/soft x-ray synchrotron, and we needed a hard x-ray synchrotron, and we needed a new neutron source. That was followed, or almost simultaneous, with the Seitz-Eastman report by the National Research Council, which was a nationwide look at the major facilities for material sciences and related disciplines. This report established priorities for the nation for a hard x-ray machine, a steady-state neutron source, a magnet lab, and improvements. Out of that report came the cold source and guide hall for the National Institute of Standards and Technology (NIST) because the report stated that the country should upgrade existing reactors. The vision that we had within the Division of Material Sciences culminated in the recommendation for the 1996 internal review budget to move forward. To achieve this vision, a decision memorandum cited ALS at Berkeley, APS at Argonne, the neutron source at Oak Ridge, and a nuclear physics facility at Brookhaven.

From the standpoint of materials sciences, we have a 667 batting average. We built two of the three. That is not bad and beats Ty Cobb's batting average by almost twice as much. We are still working on the third one because our need for neutrons has not changed. We have just hit a little snag in the road. Energy Research has commitments to its laboratories in exactly the same way as DP. The decision memorandum cited these facilities because they contribute to the vitality of the ER laboratories and to the nation, not in a national security sense, but economic security, energy security, and so forth. The year 1996 calls for a spallation source with Oak Ridge still as the preferred site, which follows the vision that we established in 1984.

The Long-Pulse Spallation Source at LANSCE

Defense Programs is considering the accelerator production of tritium (APT). I think that an important component of APT would be the long-pulse spallation source (LPSS) here at Los Alamos. This source would be important for the research and development (R&D) of accelerator-produced tritium and would also be important for R&D on targets for spallation sources, not only in this country but also in Europe. No other place can deposit that kind of energy. I would urge you, for whatever it is worth, to proceed with LPSS. It also explores a new region for producing neutrons. It is different from a short-pulse source, which de-

posits energy very quickly and where you want to get very high peak intensities. The LPSS is similar to what the Swiss are doing at much lower energy. They still have not been able to get their target design to work, so they have had to back off.

I have given you the vision; it has not changed. It is the same vision we had before—the nation needs neutrons. We can succeed. The laboratories can work together. The nation needs strong neutron science capability. Squabbles, if I can borrow something from DP, among the laboratories can only lead to mutually assured destruction. I think we should try to work together to meet the needs of the nation with this important capability.

Los Alamos National Laboratory Strategic Directions

*S. Hecker, Director,
Los Alamos National Laboratory*

Introduction

It is my pleasure to welcome you to Los Alamos. I like the idea of bringing together all aspects of the research community—defense, basic science, and industrial. It is particularly important in today's times of constrained budgets and in fields such as neutron research because I am convinced that the best science and the best applications will come from their interplay. If we do the science well, then we will do good applications. Keeping our eye focused on interesting applications will spawn new areas of science. This interplay is especially critical, and it is good to have these communities represented here today.

I would like to talk about strategic directions at the Laboratory. In the spirit that today is neutron day, I would like to show you how neutrons fit into the strategic direction of the Laboratory. As Vic Reis pointed out, a year and half ago we were looking at diversification as part of the strategic plan of the Laboratory. Because of Vic's urging during that time and because we had the Galvin Task Force process helping to establish the futures of the Department of Energy (DOE) laboratories, we have had good occasion to go back and see what has made this laboratory successful and what lessons we have learned that might help us to guide the future.

A Compelling Mission through History

We felt two things were crucial as we looked into our 51-year history. One, you have to have a compelling national mission. Two, you have to have great science because the missions for a national laboratory tend to change over time and you need the flexibility to meet those changes. If you strictly focused on an application and that application changes, you drop off the end of the earth. We have been and still are fortunate because the Laboratory has a great science underpinning. It was founded on the basis of great science with

J. Robert Oppenheimer and his colleagues when they came here during the Manhattan Project.

During the Manhattan Project, in retrospect, the compelling national mission was simple and that was to build the first atomic bomb. During the cold war, it was not quite as straightforward, but still reasonably simple and that was to redo the nuclear weapons technology to provide for deterrence against a rather capable adversary. Now we ask what is the compelling mission for laboratories such as Los Alamos as we look into the future? The answer is the theme of reducing the global nuclear danger.

To avoid just playing to a slogan, we tried to build our new theme into an actual program. I have broken it up into the following five pieces:

- stockpile stewardship
- stockpile support
- nuclear materials management
- non- and counter-proliferation
- environmental stewardship

To some extent stockpile stewardship has been made somewhat easier because we are going to have many fewer weapons to look after and even fewer weapon systems. However, it has been made harder because we will no longer be able to test. In our case, the "underground" truth is that nuclear testing has been the cornerstone of the way that we developed nuclear weapons and took care of nuclear weapons.

The Department of Defense (DoD) has not asked for new weapons. The ones we have designed will have to stay in the stockpile much longer than originally anticipated. If you need more weapons in the future, where do you get them? The current weapons complex is clearly oversized to perform that mission in the future. If we are going to keep these weapons in

the stockpile decades longer than we designed them for, we have a different problem than we had before. In addition, we cannot test and must understand these weapons better than we have ever understood them, which is the rationale for science-based stockpile stewardship (SBSS).

Gaining Confidence in the Weapons Stockpile

Peter Jones, the former director of the Aldermaston establishment in the United Kingdom, said one has to remember that the safety of the weapons rests in the people and not in the product. Another way of saying this, the confidence and the safety of the weapons rest in the people and not in the product. Just delivering the product to the military does not assure a safe, secure, reliable deterrent for the country. Therefore, the confidence in nuclear weapons equals the vitality or the confidence in the Laboratory.

Stockpile support essentially integrates the research and development (R&D) and the manufacturing or disassembly capabilities of the nuclear weapons complex, which has only been possible in the past couple of years. Much of our effort now is aimed at ensuring that the disassembly is done in a safe and reliable fashion and that those products that go away, such as tritium because of radioactive decay, are replenished. We have come up with the concept of producing tritium with accelerators. We have proposed to use the accelerator to make neutrons in order to make tritium, which becomes part of stockpile support.

The investment that the government has made in Los Alamos for over 50 years and the expertise that we have contributes to our mission. One piece in our mission is nuclear materials management. In 1941, plutonium was the answer, and today to a large extent, it is a problem that someone has to solve. Some 13 tons of plutonium is at Rocky Flats in a form that you cannot keep there because Colorado citizens do not want it, but you cannot get it out of there either. Rocky Flats has been shut down for 5 years and everything is sitting there in suspended animation. Only places such as Los Alamos and Livermore have the

capabilities to do something about the material. To get rid of plutonium in the long term and to mine some of the energy out of it becomes a significant problem. Neutrons will play a role.

Non- and counter-proliferation has clearly become a major issue. They are very tightly connected because being able to count the number of nuclear weapons is reasonably straightforward in a place like Russia. However, accounting for where the nuclear material is or has been for all of these years and then how to make sure that nuclear material is actually safeguarded and eventually disposed of are major problems. We have some major initiatives with our former adversaries, the Los Alamos and Livermore equivalents in Russia, to work together on nuclear materials control and accountability. They had no nuclear materials control and accountability system using modern technology. They did it strictly by armed guard. If you put your arms around the complex, the plutonium does not get out. As you know, the arms are coming apart. We are demonstrating at Arzimas 16, their Los Alamos, the first nuclear materials control and accountability system. A few weeks ago, Sandia demonstrated at a Russian civilian institute one of the physical protection systems that they had been developing over the year. Our laboratories are playing an important role in the issues at the top of the national security agenda today.

Environmental stewardship is cleaning up the legacy of 50 years as part of reducing the global nuclear danger because many folks in this country think that this is the nuclear danger. However, at our laboratory we worry about all aspects of nuclear danger. We think that this is a legitimate compelling mission for a place such as Los Alamos.

Working within a Tight Budget

When estimated dollar signs are put on fiscal year 1995, the five pieces are all significant in making a program (Figure 1). If we had a compelling central mission with close to 700 million dollars, I would say that our laboratory would be in good shape. However, we are now starting to integrate this stockpile support

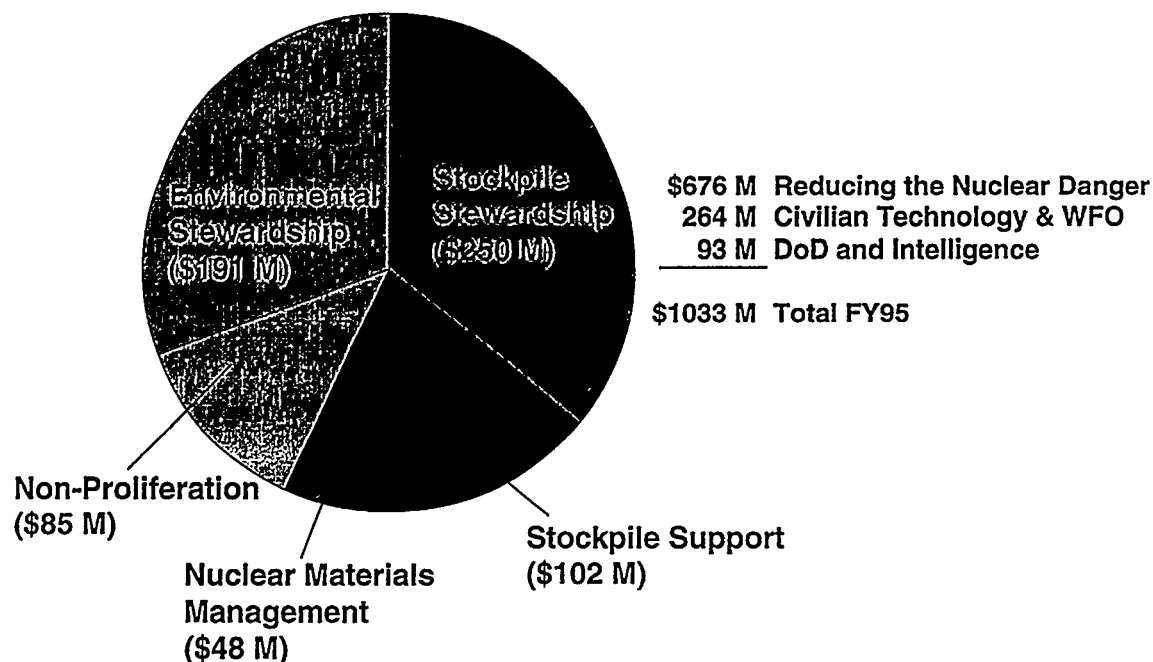


Figure 1. The five pieces for reducing the nuclear danger are all significant in making a program. Estimated dollar signs are for fiscal year 1995.

into our central mission. For the rest of these pieces, we get our funding in tea cups, rather than in truck loads. They are not as well integrated, certainly at DOE Headquarters, as they would need to be to make this a central compelling mission, but we are working on it. However, to do the core mission right, you need science in the core technical competencies and must nurture those core technical competencies. You have to build an environment in the Laboratory where you attract the best scientists in the world in a broad range of disciplines.

In the past, we have said that we are also a multiprogram laboratory that works for DOE. If the nation keeps us at the top of the game in certain areas of science, then we should be able to use that expertise to help in other areas. For instance, we are one of the principal players in the Human Genome Project because we were the first, along with Lawrence Livermore, to look at computational biology using the enormous computational resources developed for defense purposes. We set up the GenBank at Los Alamos and Livermore, and that evolved into our expertise in the human genome. We also developed laser flow cytometry, which was also refined at Lawrence Livermore. We were able to add something

special because we could apply our expertise in physical sciences to life sciences. We have picked civilian, industrial, and defense problems to solve on the basis of our expertise.

In our changing world, it is not just an issue of us providing some expertise to the outside world. We think that this outside world has to contribute to the vitality of the science base here. The interchange with the energy research community is extremely important for us to stay at the top of our game. The industrial partnerships were questioned in the Galvin report. However, this interchange is an absolute necessity. Whether it is SBSS or manufacturing of the future, we must work with American industry to get all the smarts we can from them, not just for them to benefit from our smarts. This interchange with the industrial world, the Pentagon, and the civilian missions is imperative for us to stay a top-rate Laboratory.

Tactical Plan for Los Alamos National Laboratory

Because Vic Reis was worried about diversification and his labs going in all directions, we have put together a tactical plan for the Labo-

ratory (Figure 2). The plan includes the things we really need to pull off in order to achieve this vision of the future. Those tactical planning goals are SBSS; the neutron lab; the plutonium legacy; great science; high-performance computing, modeling, and simulation; and the industrial partnerships.

To meet the stockpile stewardship requirements, great science and a computational focus are important. I want to explain how keeping weapons in the stockpile longer taxes our ability to understand materials, why materials become more important, and why neutron scattering or neutron radiography become important to nuclear weapons and SBSS. The aboveground experiments are key and that is where the Los Alamos Neutron Science Center (LANSCE), the National Ignition Facility, our Dual-Axis Radiographic Hydrodynamic Test (DARHT) facility, and our Argonne Tandem-Linac Accelerator System (ATLAS) pulse-power facility become important. We also need a greater integration of weapons scientists and engineers into the research community. We have always had the people in our theoretical, physics, and life sciences divisions fully integrated into the national research community. However, a good part of our weapons program has naturally been more confined.

Studying Plutonium with Neutrons

Neutrons spurred the initial interest in plutonium. But all those in chemistry, materials, and other fields know that the electrons are what really count. Eventually you will need neutrons to figure out why the electrons, especially in plutonium, are doing such funny things. I thought that I would tell you about this interesting thing called plutonium.

Plutonium melts at 641°C and does some incredible things along the way. If you compare

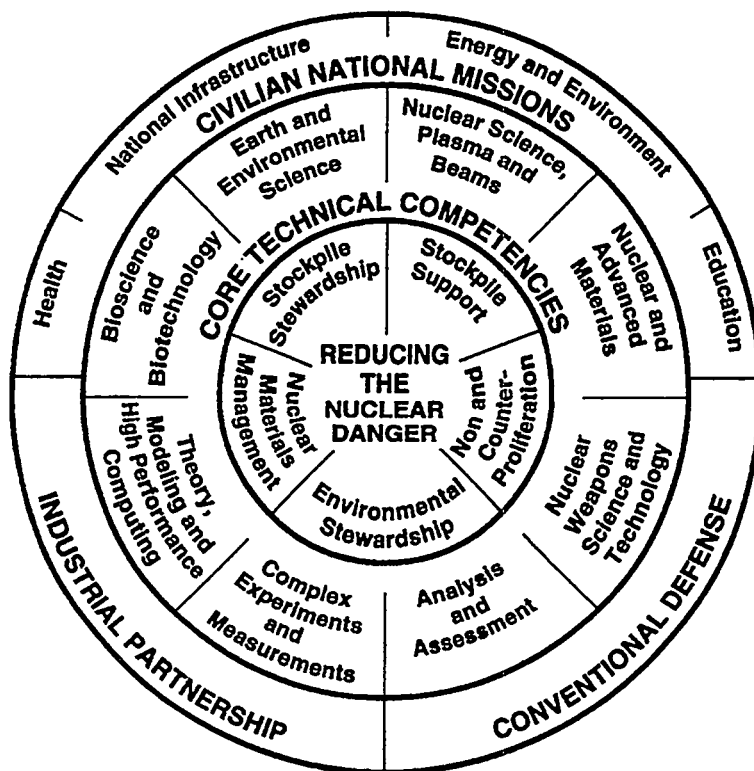


Figure 2. At Los Alamos, the central mission of reducing the nuclear danger supports a set of core technical competencies that allows us to contribute to civilian and industrial needs. In turn, the intellectual challenges of civilian and industrial problems allow us to strengthen the core competencies for the defense missions in an era of declining resources.

it to something most people think is really complex like iron and then look at the density changes, you can see the volume change is about 13% (Figure 3). It is also quite easy to go directly from the delta phase to the alpha phase and vice versa, which gives you a 20% volume change. You are dealing with a solid that undergoes a 20% volume change when you barely look at it. You might imagine what happens when you squeeze it. The crystal structures are ones that I can only now appreciate. The only thing that I have seen that is more difficult is in the biosciences when you start looking at protein molecules. A simple monoclinic system is difficult for most metallurgists to work with.

If you look at plutonium on the periodic table in the actinides, you find that it does some very peculiar things. Where you might have expected the melting points in the transition elements to go up as you go across the table,

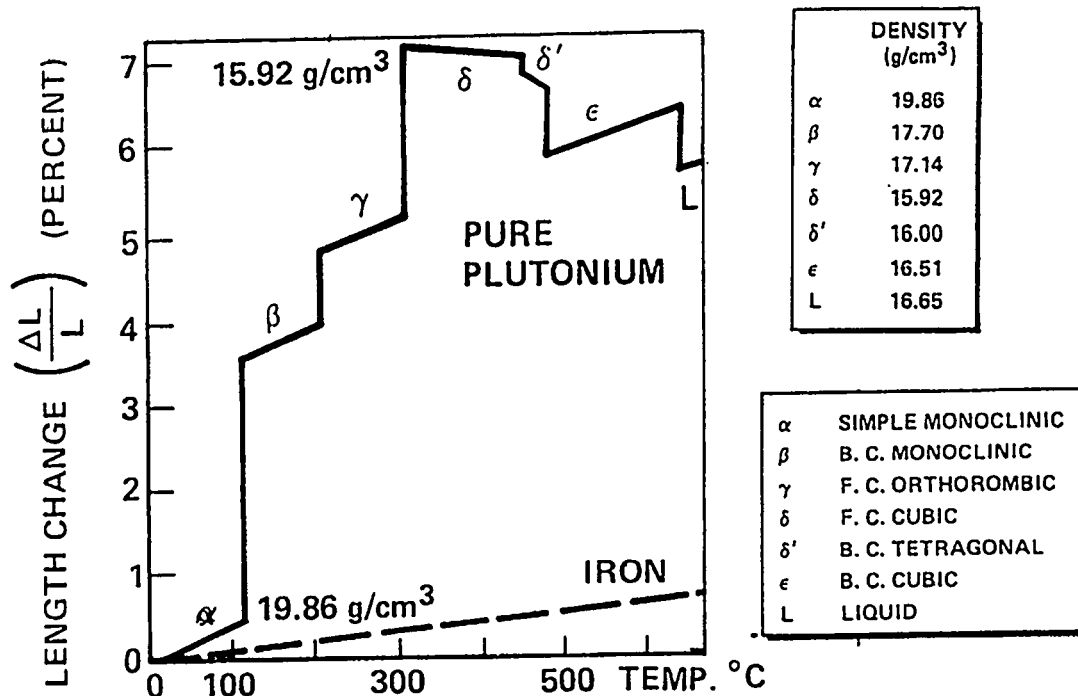


Figure 3. The practical consequences of 5f electron bonding—thermal instability and low melting point.

you can see that in plutonium it drops down and has this anomalous low melting point (Figure 4); it has six crystal structures. If you alloy it with almost anything, particularly with things like aluminum, gallium, americium, you can stabilize the delta phase reasonably easily. The delta phase is cubic and that is what metallurgist like to work with. We know how to make things out of it. The point is it takes a rather little alloying to change the plutonium.

A few years ago, Jim Smith from this Laboratory took the liberty of rearranging the periodic table. He put the 4f series above the 5f series to get a rather interesting alignment of the periodic table (Figure 5). We seem to have a boundary or a region that separates the place where you have localized electrons and get magnetic behavior from where you get the electrons in a bonding mode and you have principally superconducting behavior. He said this boundary contains most of the elements—cerium, neptunium, plutonium, manganese, iron, and so forth—that are an irritation in life. They have lots of phase changes; they do all kinds of strange things. He said we can play many material solid-state physics games by squeezing these elements, and things may

change from superconducting to a magnetic behavior. Also, we can alloy them to expand the lattices.

At this Laboratory in the 70s and 80s, scientists tried to understand the influence of the 5f electrons particularly on plutonium recognizing that almost any little thing that you do to it will change its behavior. The crystal structures and the behavioral changes are enormous; it is not just a matter of having a small difference in thermal expansion coefficient. Now, in addition to this problem, which we looked at for the sake of good science, we also looked at it from an alloy development standpoint when we were still trying to develop better alloys of plutonium. No one cares today if you have better alloys of plutonium, but people care that those alloys in the stockpile are going to stand up to the test of time.

Plutonium decays through alpha decay. The 239 isotope takes 24,400 years to decay, and its half-life is 24,400 years. Nevertheless, the alpha decay eventually makes helium bubbles. Some years ago, we had an absolute tour de force in metallurgy at this Laboratory because we were able to do transmission electron

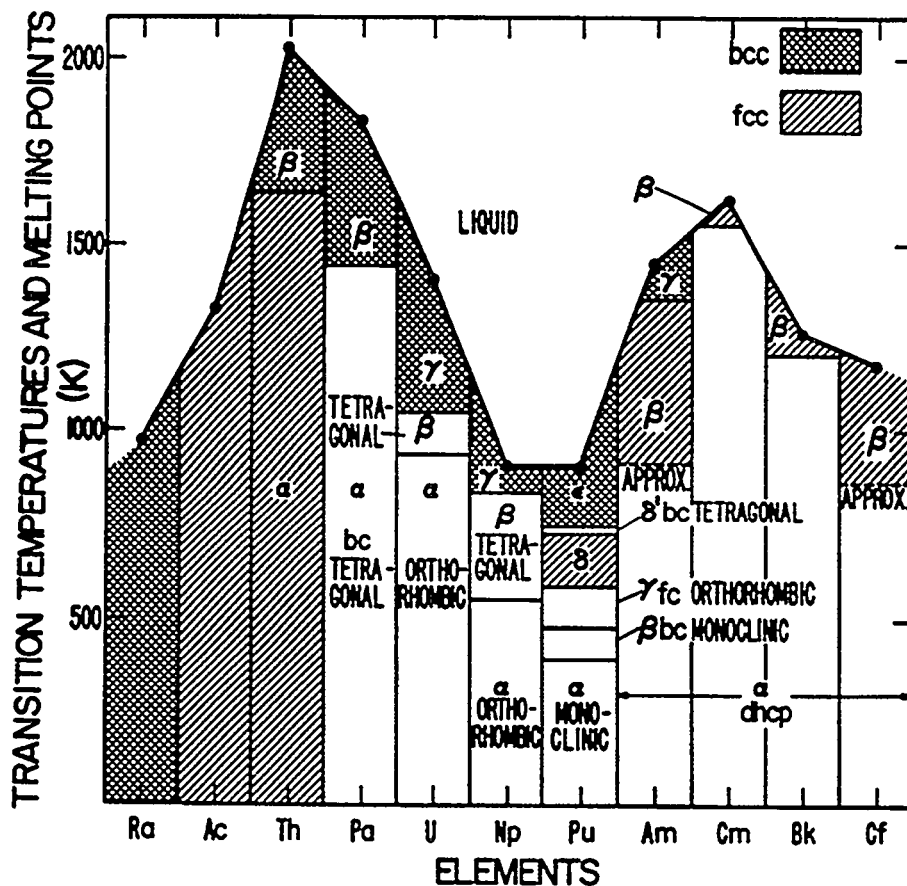


Figure 4. As you go across the table, the transition temperatures and melting points of the elements drop at plutonium.

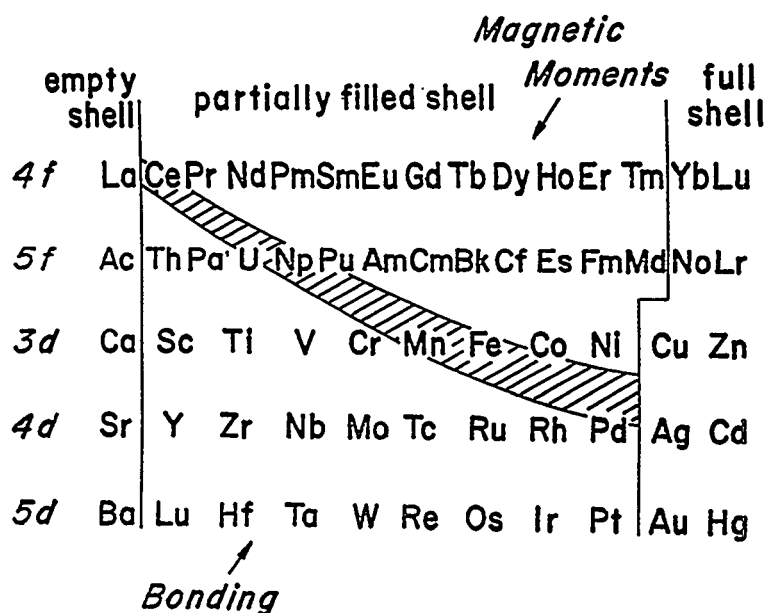


Figure 5. The 4f series is above the 5f series on this periodic table.

microscopy of plutonium, which oxidizes more ferociously than any other element on the table. We could look at helium bubbles in a 20-year old, very pure plutonium sample. We stopped this program a few years ago because we could not justify it on the basis of our nuclear weapons budget. Today we will restart it. Those of you that are neutron experts understand that the real way to look at the bubbles and to look at voids is to use small-angle neutron scattering.

Because of the decay of weapons-grade plutonium, you grow in americium as a function of time. When you kept the weapons in the stockpile for 20 years, nobody cared, but if you are going to keep plutonium in a pit for 40, 60, 80 years, then you start asking questions. In a similar way, you can ask questions about what happens to the high explosive? Of course it does not have a half-life, but it is a lot worse than plutonium. You have to worry about grain boundary corrosion; you need to be concerned about a whole slue of stockpile issues. In fact, we have put together for the defense programs effort experiments you can do at LANSCE in the future to support SBSS.

For the plutonium legacy, I want to review the plutonium road map and why neutrons are important (Figure 6). To get to a world where you have gotten rid of most of the plutonium and want to extract the energy, you will need neutrons from a reactor or an accelerator. We thought of things such as plutonium burning or waste transmutation with accelerators. We are looking at plutonium lifetimes, and we are concentrating on securing and stabilizing the plutonium. Eventually we will have to store it. That is a problem that Los Alamos is very interested in. Neutrons play an important role in the technology.

LANSCE Provides a Vital Service to the Nation

If you use the accelerator and have an intense neutron source, you can do materials research, tritium production, plutonium disposition, waste transmutation, or energy production if you feed in a little natural uranium or thorium. The great science part is that we see LANSCE as being essential to the scientific vitality. We know we can do the stewardship and the integrated role depending on the exact require-

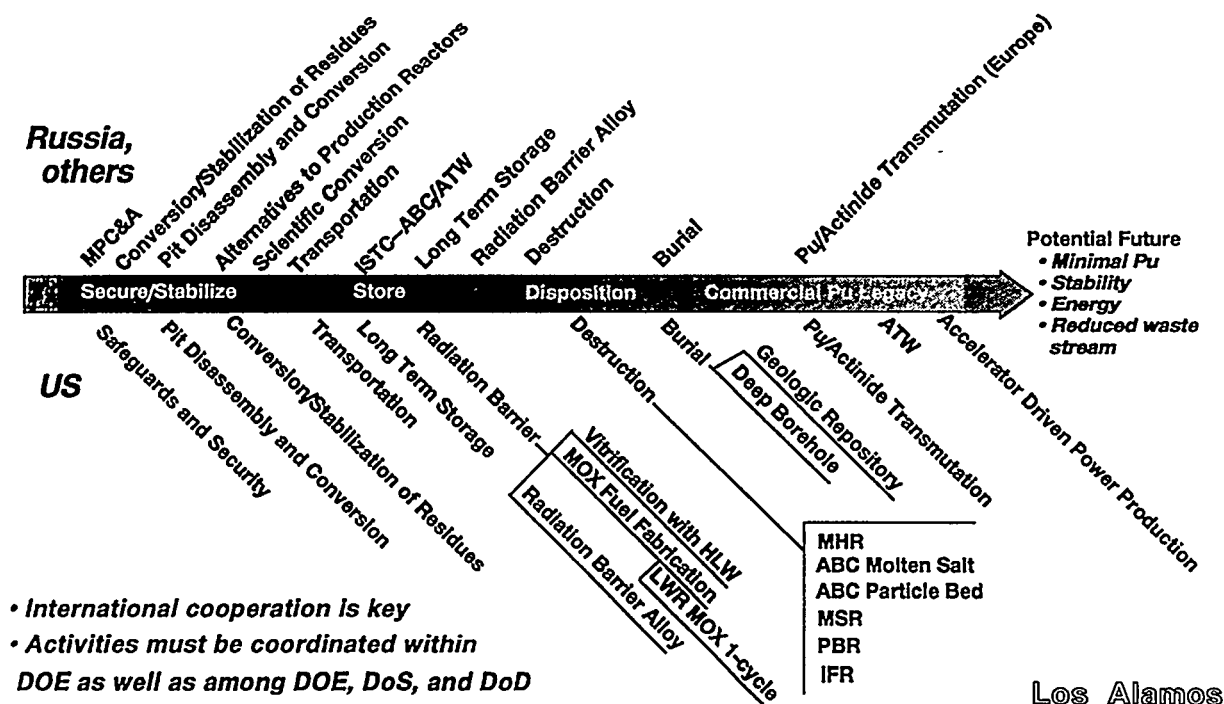


Figure 6. The Los Alamos Neutron Science Center can play an important role in the plutonium road map.

ments. The question is how do we make sure that we keep a focus at this Laboratory that attracts the best of the scientists and gets us intermixing with the scientific community to keep this Laboratory as a vital service to the nation? LANSCE has these components.

Whether we have done materials research on superconductors, structural biology, or fundamental work in physics, this accelerator is really important to research at Los Alamos. It is the best neutrino source in the world. We have recently reported that it appears we have evidence for neutrino oscillations.

Let me say a word about high-performance computing and how it fits in. One of the things that we have always liked about a spallation neutron source compared to reactors is that we feel spallation neutron sources are just at the beginning of their utility. We can get more out of a spallation source if we really apply the computational horsepower of a

place such as Los Alamos for time-of-flight neutron scattering work. I would like to see us contribute this capability to that community to really beef up neutron scattering.

The industrial goal is one that we have worked, and we have actually developed industrial partnerships over the past 10 years as part of the Strategic Defense Initiative program, neutral particle beam, free-electron laser program, and now looking at the accelerator production of tritium (APT), working very closely with industrial companies.

The neutron laboratory is probably best captured by the spallation neutron road map that John Browne and Roger Pynn put together (Figure 7). LANSCE has never lived up to its expectations. It was a parasitic facility the Clinton P. Anderson Meson Physics Facility (LAMPF). Running a user facility for the nuclear physics community was the first priority. We made the decision a few years ago that we

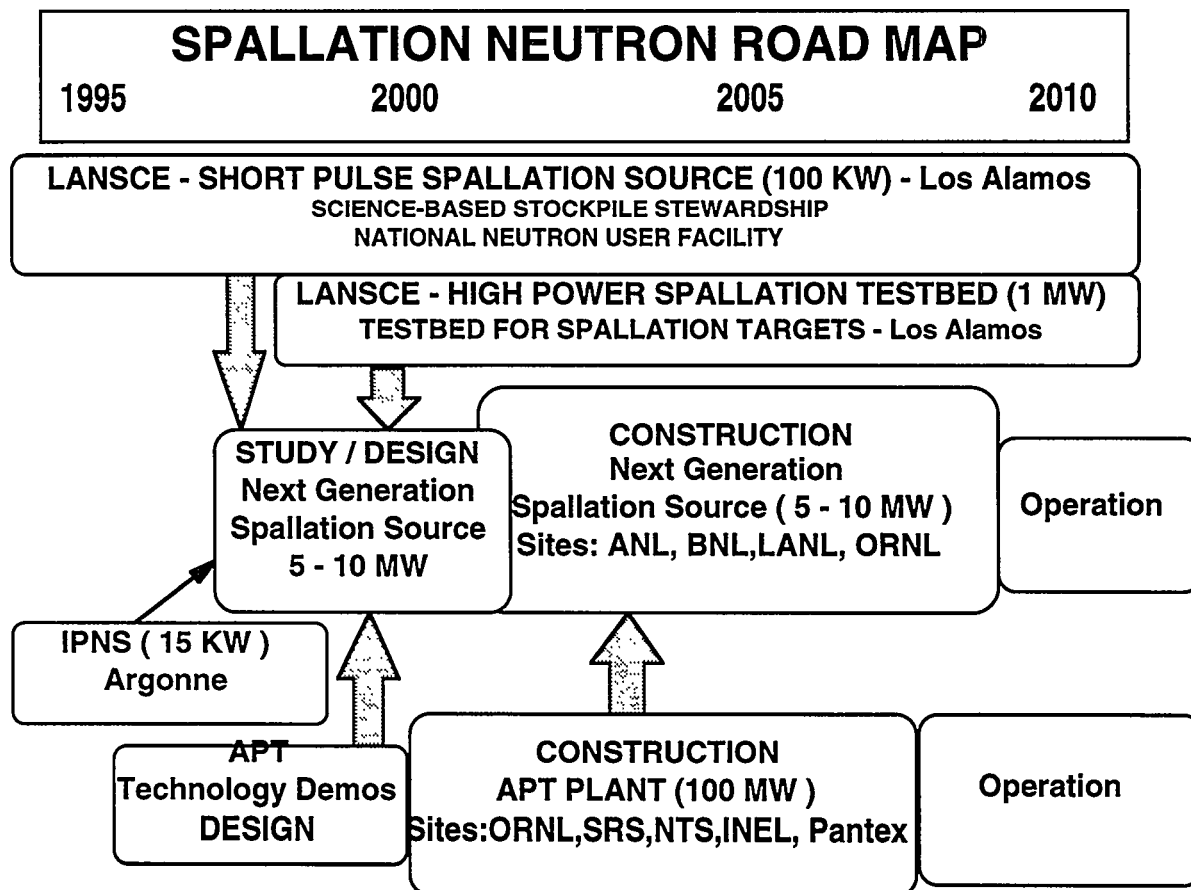


Figure 7. The spallation neutron road map shows the relationship and time scale of various projects that contribute to the construction of a next-generation spallation source.

were going to change our priorities and go with LANSCE. We got help in fiscal years 1994 and 1995 to upgrade LANSCE so that we can reliably run it and provide good availability. We want the material and biological communities to say Los Alamos is a good place to come and do research. Running LAMPF 3 months a year did not excite the materials community. If I am working with plutonium or something else, I am not very satisfied if I have to come back a year later. We need availability 8 months a year. We have made the decision and the commitment that we are going to give the country the best spallation source for the next 10 years or so with this LANSCE upgrade. We have committed to have neutron scattering at Los Alamos.

In addition, the APT program, if accepted as the technology of choice, will need to run over the next 3 to 4 years to allow us to develop accelerator and target capabilities that should then help with looking at the future of spallation neutron sources. Fortunately, there is \$25 million in the budget from the Office of Defense Programs to support SBSS and around \$7 million from the Office of Energy Research (ER). It will be a real challenge to provide the neutrons in 1996 for that kind of money.

Neutron Sources in the Future

While there was still the possibility of having a reactor and a spallation source, we had been looking, along with Argonne, at next-generation spallation neutron sources. Lee Schroeder from Lawrence Berkeley Laboratory has been heading those efforts and looking at spallation neutron sources for the future—what we call the short-pulse spallation sources. In the meantime, our people with some people from Europe thought of running the proton beam directly into the target and building this long-pulse spallation source for making neutrons available as well as having it

as a testbed for target work. This makes sense only at Los Alamos because we already have the 800-MeV proton accelerator here. In addition, the other interests of Los Alamos are the accelerator-related transmutation technologies such as waste transmutation, plutonium burning, and so forth.

We hope to provide the neutrons needed for our programs and the defense program, but also through partnerships provide neutrons to the materials and biological research communities as well. In the fiscal year 1996 budget, we did not anticipate that a laboratory would be chosen for the spallation source that was not a proponent of spallation sources and had been touting the reactor for some time. It is not clear right now what a conceptual design of a spallation neutron facility needs to be—do you build a 1 megawatt, do you build a 5 megawatt, and if you build a 5 megawatt, where are you going to do the target research. We have the idea of doing a long pulse. At this point, we would like to see the community get together because a major milestone has been passed. For better or worse, the reactor at this point is dead, and we need to concentrate on spallation sources. We think that the most important thing that is commensurate with typical procedures at Basic Energy Sciences and ER is to make sure that there is appropriate peer review of the concepts for the spallation source that may eventually go to Oak Ridge, Argonne, or Los Alamos. The institutional factors will clearly need to be factored in at some point, but we cannot do that in my opinion at the expense of doing the peer review on the technical ideas.

I tried to give you an idea of where Los Alamos is going. Neutrons are a big part of our future. We will work with the research community to provide neutrons so that you can help stimulate us to make sure our science is good and then to make sure we do our defense responsibilities.

Science-Based Stockpile Stewardship at Los Alamos National Laboratory

*J. Immele, Director, Nuclear Weapons Technology Programs,
Los Alamos National Laboratory*

Introduction

I would like to start by working from Vic Reis's total quality management diagram in which he began with the strategy and then worked through the customer requirements—what the Department of Defense (DoD) is hoping for from the science-based stockpile stewardship program. Maybe our customer's requirements will help guide some of the issues that we should be working on. One quick answer to “why have we adopted a science-based strategy” is that nuclear weapons are a 50-year responsibility, not just a 5-year responsibility, and stewardship without testing is a grand challenge. While we can do engineering maintenance and turn over and remake a few things on the short time scale, without nuclear testing, without new weapons development, and without much of the manufacturing base that we had in the past, we need to learn better just how these weapons are actually working.

Meeting the Customer's Requirements

The customers—the national security apparatus, the White House, the joint chiefs—are looking for confidence, as well as weapons judgment, among other things. The national laboratories work together on one national program, but this one program includes the spectrum of activities ranging from basic research, applied research, and dealing with stockpile problems. Weapons judgment is going to require familiarity with integral systems, even including gaps and cracks and little imperfections that matter in nuclear weapons. With neutron scattering, we are looking at a tool that can provide information about some of those systems, even at the metallurgical scale, and tell us what is going on. This information can be integrated back eventually to making a judgment about the performance of the weapon.

Working backward from the customer requirement, I would like to discuss the following six pillars of the weapons program, as we call them, that summarize the issues that we have to address:

- weapons performance
- weapons science
- enduring stockpile systems
- post cold war uncertainties
- surety
- factory of the future

I think that I can explain to the joint chiefs of staff why every one of these six pillars matters. I would like to begin with a few examples of where neutron scattering is going to make directly relevant contributions, which I can relate back to the customer—the joint chiefs of staff, national security apparatus, the White House, and so forth.

We can use neutron scattering for surveillance. I will remind you that we now think of an enduring stockpile as one that does not turn over in 25 or 30 years but may go several cycles of those 25 or 30 years. Whether we may re-qualify or replace parts is going to depend on our assessment of the materials—how they are aging and how they are going to perform if they have changed a little bit. Plutonium is as an example.

Weapons science refers to understanding how things happen. Hydrotesting is the most important aboveground experimental technology. Most of the problems with reliability and safety in the stockpile have occurred with the primary, so understanding how that works is critical. Let me pose a challenge to you. What is happening metallurgically after we shock old plutonium? We do not have plutonium that is 60 and 90 years old yet, but eventually, we are going to have to understand old plutonium. (We are thinking that maybe we can get Sig back on the bench to artificially age plutonium

past the date that it was originally introduced to the planet.) Shocking the plutonium can affect the compression of the material. The challenge to all of those in the neutron scattering community is to design some experiments that will give us some insight into this question.

Changes in the Nuclear Weapons Program

Activity at Los Alamos and other laboratories has diminished considerably in the area of developing enduring stockpile systems. In fact, M. R. C. Greenwood mentioned that among the spectrum of basic applied science and development, it is development where the government has put the emphasis on reductions that have happened here. Our weapons program budget is down by 55% from what it was in 1987 and most of that is in the development area. Nevertheless, we are still going to have to learn how things get put together into a full item.

Let me mention just one post cold war uncertainty, which is proliferation. Within nuclear physics, there are threshold fissioners, things like neptunium 237, which may have considerable proliferation potential but are not currently controlled. How we do materials control and accountability in the future is an issue.

With active interrogation, as well as passive detectors, the experimental nuclear physicists can make contributions to this area as well.

Surety refers to how we are going to have to understand how explosives respond. Our plastic-bonded explosives initiate under a shock wave influence because of the shearing of crystals, which forms hot spots. Under low impetuses, we want to understand how the hot spots form and what the reactions are chemically. The short-pulse spallation source will be able to provide us with a snapshot of what is going on with the crystal shearing and the beginning of the chemical reactions.

With the factory of the future, I think that we can make a loop back to the surveillance of nuclear weapons. We are going to requality many things. When we do remake things, we are going to have to make them with much lower amounts of waste than before, and therefore, the processing will be different. We are going to have to understand the material processes as the materials age, as the materials are shocked, and as the materials are remade into new things.

This is the quick summary of the areas, from the point of view of the customer, that we can apply neutron scattering to in very direct and relevant ways.

Science-Based Stockpile Stewardship at LANSCE

*J. Browne, Director, LANSCE and Energy Research Programs,
Los Alamos National Laboratory*

Introduction

Let me tell you a little about the Los Alamos Neutron Science Center (LANSCE) and how some of the examples you heard about from Sig Hecker and John Immele fit together in this view of a different world in the future where defense, basic, and industrial research overlap. I am going to talk about science-based stockpile stewardship at LANSCE; the accelerator production of tritium (APT), which I think has a real bearing on the neutron road map; the world-class neutron science user facility, for which I will provide some examples so you can see the connection with defense science; and lastly, testing concepts for a high-power spallation neutron target and waste transmutation.

LANSCE and its Associated Facilities

It is important to understand LANSCE to appreciate the related projects. First of all, Los Alamos has a high-power proton linear accelerator (linac)—800 MeV, and a little over a mA for essentially 1 MW of power in the beam (Figure 1). It has been the highest power proton linac for the last 25 years and has operated with high reliability during that period. The area at the end of the linac is where the medium-energy nuclear physics has been done. About 15 years ago, we recognized the importance and value of this facility for producing spallation neutrons. We were able to take a portion of the beam under the road over to the Manuel Lujan Jr. Neutron Scattering Center. The Proton Storage Ring, which was built between 1980 to 1985, compresses the pulse out of the linac down to a pulse of about 270 nsec, which is good for producing neutrons in the thermal and eV resonance range.

We have several different capabilities for neutron production. One capability is what I have called a very short-pulse spallation source (VSPSS) because you can see that the time structure is less than 1 nsec. The VSPSS at the

Weapons Neutron Research (WNR) Facility uses a microstructure out of the Clinton P. Anderson Meson Physics Facility (LAMPF) beam. The neutron energies that we typically create with spallation are in the energy range of about 1 MeV up to around 600 MeV. The very high frequency, 18 kHz of the VSPSS, is fine for high-energy neutron research. At the VSPSS, we can do high-energy neutron radiography, which is something very new that we have been exploring. Traditionally, nuclear data has been collected at WNR, and it is very important for this new world without nuclear testing. We have done target moderator studies, which have allowed us to benchmark the codes that we used to develop target moderator systems for the Neutron Scattering Center. We have done some very nice work in the area of materials irradiations, which used protons as well as neutrons. There also has been a lot of fundamental nuclear physics carried out at WNR.

At the short-pulse spallation source (SPSS), which is our Manuel Lujan Jr. Neutron Scattering Center, pulse lengths are determined principally by moderation, and the energies of the neutrons likewise in the 10-meV to approximately 1-eV range, and we are running about 20 Hz. The types of experiments that we have done are powder/single-crystal diffraction, thermal/epithermal neutron inelastic scattering, and fundamental physics. We would also like to do resonance radiography, which John Immele talked about, for questions of high explosives, particularly looking at resonance radiography in a dynamic sense. A single pulse out of the Proton Storage Ring can give us enough data that we can measure resonance absorption and look for the Doppler width. As a result, we get a temperature of something occurring dynamically in a high explosive. This is very important for hot spot initiation questions and our models of high explosives.

The Los Alamos Neutron Science Center

2 kW VSPSS

$\Delta T < 1$ nsec; $1 \text{ MeV} < E < 600 \text{ MeV}$; 18,000 pps

- high-energy radiography
- nuclear data
- target/moderator studies
- materials irradiations
- fundamental nuclear physics (e.g. nucleon-nucleon)

High-Power Proton Linac
800 MeV; 1.2 mA

Experiment Hall

- neutrino oscillations
- other "high-priority" nuclear physics experiments
- *APT-related experiments*
- radioisotope production

1 MW LPSS

$\Delta T \sim 1$ msec; $E \lesssim 10 \text{ MeV}$; 60 pps

- high-power spallation target test bed
- high-energy neutron radiography
- diffuse scattering
- SANS
- NSE
- reflectometry
- cold-neutron inelastic scattering
- Laue diffraction
- UCN

80 kW SPSS

$10 \mu\text{sec} \lesssim \Delta T \lesssim 100 \mu\text{sec}$; $10 \text{ MeV} \lesssim E \lesssim 1 \text{ eV}$; 20 pps

- powder/ single-crystal diffraction
- thermal/ epithermal neutron inelastic scattering
- *resonance radiography*
- fundamental physics (e.g. parity violation)

Figure 1. The present and future facilities at LANSCE and their associated research capabilities (future facilities and capabilities are in italics).

Because the nuclear physics program will complete its program at the end of this fiscal year, the whole 1-mA beam is available for other neutron research. Right now we are looking at and studying the 1-MW long-pulse spallation source (LPSS), which has a very, very long time structure—1 msec—and the energies of the neutrons that you might look at are going to be much less, much more like what you would do with a cold neutron source or even ultra-cold neutron source. We have not done anything with the capabilities associated with the LPSS, but it is clearly a place where we could have a high-power spallation test-bed and do various experiments, including experiments that are very key for accelerator production of tritium or testing concepts of transmutation of waste.

We are upgrading the accelerator now. We started last year. The principal goal of this 35-million-dollar improvement program is to improve the reliability so we can provide the users with 85% reliability with respect to schedule. We are also making it capable of running 8 months per year. We are looking at some different injection schemes through the Proton Storage Ring to get the beam current up to 100 μ A at 20 Hz with the capability perhaps of going up to 200 μ A at 40 Hz, which will clearly put us in the ballpark of Rutherford Appleton Laboratory's neutron intensity. This program is under way and scheduled for completion in 1997.

Science-Based Stockpile Stewardship Research at LANSCE

One example of using LANSCE for science-based stockpile stewardship is in the area of fast neutron radiography (Figure 2). Fast neutron radiography allows you to look inside assemblies to see if they have problems—cracks, voids, and gaps—without disassembling them, and you might be able to save a lot of time and money with respect to the stockpile. The high-energy neutron beam greater than about 10 MeV passes neutrons through a sandwich in which you have several inches of depleted uranium, followed by a light material like lithium hydride, followed by another thick piece of depleted uranium. We wanted to know if by passing high-energy neutrons through those

layers, could you see voids and gaps? We simulated what we thought we could see, about a 4-mm spot and was just a proof-of-principle experiment. What we measured allows us to actually see small holes drilled in the lithium hydride after the beam passes through a very, very thick sample of uranium. We believe this capability has potential for further development. It could actually have significant impact on the surveillance programs being considered for the stockpile.

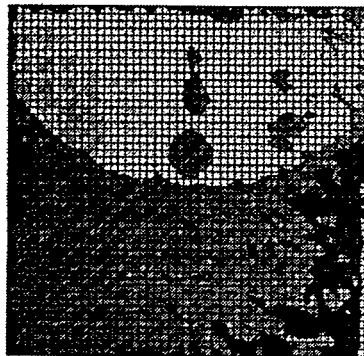
Another example that I would like to point out concerns the issue of texture in manufacturing. As most material scientists know, texture, which is the crystal orientation, does make a difference. How you manufacture something and how the texture turns out can affect the performance, which is very important in a lot of weapon components and in a lot of other materials. Figure 2 shows a shape charge liner of tantalum. Near the base of the cone you can see the preferred orientation in the 1-1-1 plane whereas near the top, the texture is more uniform. With this kind of knowledge, you can then use calculations to predict the dynamic behavior of materials.

I have a series of examples of what we have done in basic and industrial research (Figure 3) including very high-pressure cell work—10-GPa high-pressure—that is clearly going to be important to some of the questions concerning plutonium and the various phases that plutonium sees, which is of interest to both Los Alamos and Lawrence Livermore laboratories. Other examples deal with manufacturing. We did research with Ford Motor Company on stress induced in a composite brake rotor, which is very applicable to induced strain that we will have to look at as we remanufacture fewer and fewer nuclear weapons.

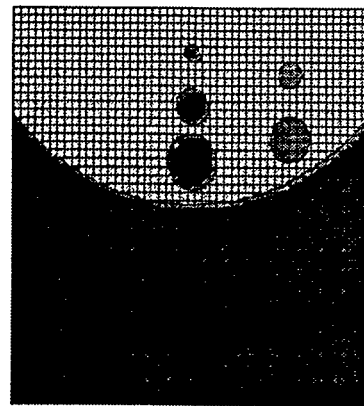
The Accelerator Production of Tritium Program and LANSCE

I want to end with a brief discussion of the APT system and what we are going to do at LANSCE. The APT system is a ~1-GeV, 100-mA device. This is a continuous-wave machine, which is very impressive. We have been reviewed about half a dozen times over the past year, and everyone has come back

Experimental



Simulation



Neutron radiography

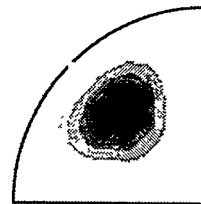
Plutonium aging



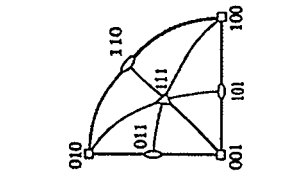
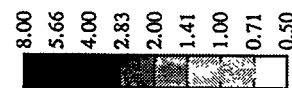
Radial Direction Inverse Pole Figures



Near Top of Cone

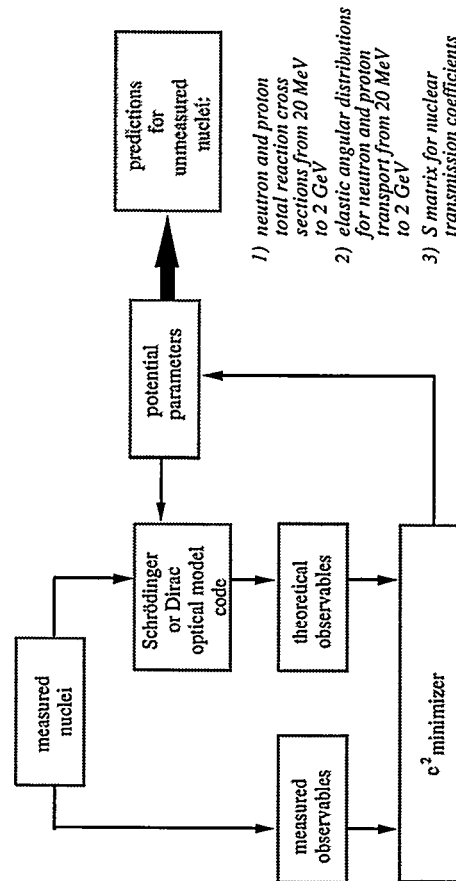


Near Base of Cone



Texture in a tantalum shape charge liner

CIC-9 d195-0096 v2



Nuclear data for SBSS
(example: OMP for APT project)

Figure 2. Examples of research performed at LANSCE that will be useful to SBSS programs.

and concluded that we can build this system. It is not a high scientific risk, but it is an engineering challenge. It certainly will have significant payback to the next-generation spallation neutron source. Assuming APT is chosen, we will be demonstrating the first 40 MeV of this continuous-wave accelerator at full 100-mA current at Los Alamos over the next 4 years. The injection end of it is the hard part. If we can get it to 40 MeV reliably at 100 mA, we really believe that the rest of the system is very straightforward.

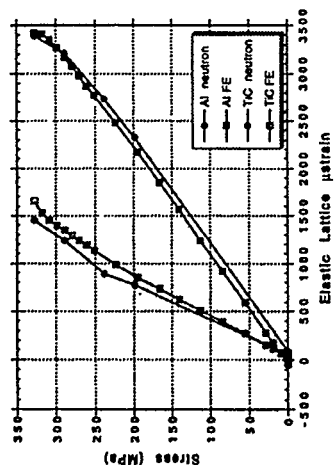
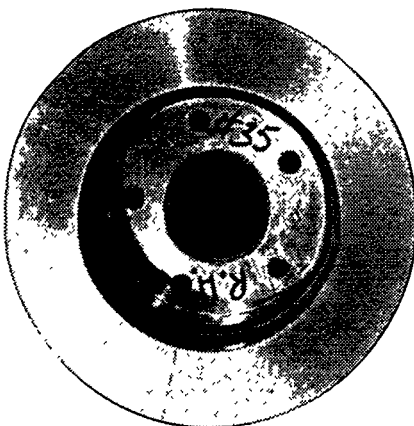
One of the questions we have concerns the target making tritium. We will be testing with the LANSCE proton beam how well we can actually calculate the number of tritons we produce with the target design we have for tritium production. This is a very key experiment. Another question we have, which I think has great overlap with the materials science community and the next-generation spallation source, concerns materials damage

at these types of fluences for proton beams and spallation neutrons. Over the last 20 years, we have had experience with a high-power beam, and we are going to have to build on that data to improve our knowledge of spallation damage so we can better understand how long these facilities will be able to operate.

The tritium system extraction facility, called the Tritium Systems Test Assembly at Los Alamos, allows you to separate tritium with very high purity. This program is important because it builds on the strengths we have and offers another opportunity to collaborate with other laboratories. We have worked with Sandia and Brookhaven on this particular program. We also see an opportunity to collaborate with Lawrence Livermore National Laboratory and other laboratories in a lot of the technologies that are important to making the APT system a reality.

Industrial Research

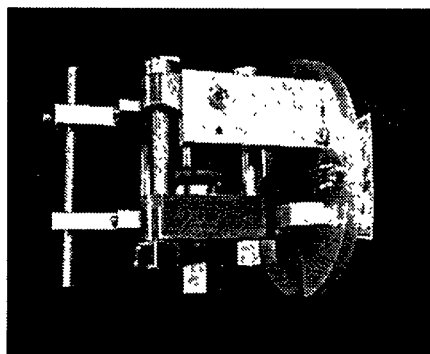
Al/SiC brake rotor



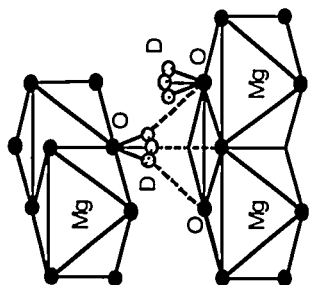
Phase strains measured in Al/TiC under load

Systems examined at LANSCE include Ti/SiC, Al/Al₂O₃ (Rockwell) and Al/SiC and Al/TiC (Ford Motor Co.)

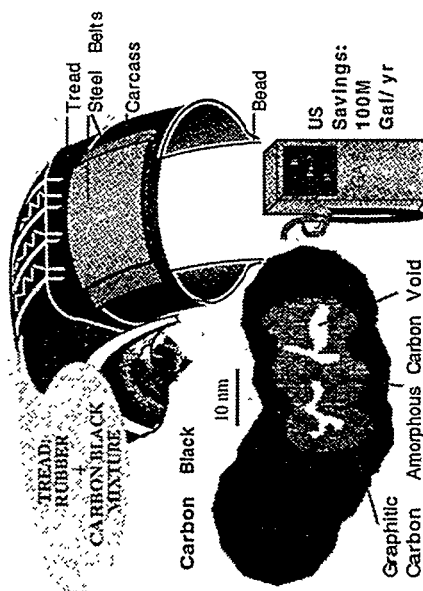
Basic Research



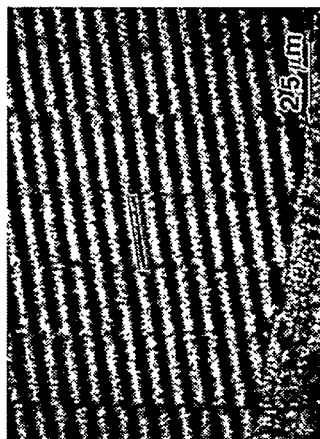
Highest pressure cell for neutron scattering in the U.S.



Structure of water bearing mineral at 100kbar.



Neutron scattering provides information on carbon black which leads to reduced tire rolling resistance, thus improved gas consumption.



Magnetic properties at thin film interfaces can be studied using polarized neutrons.

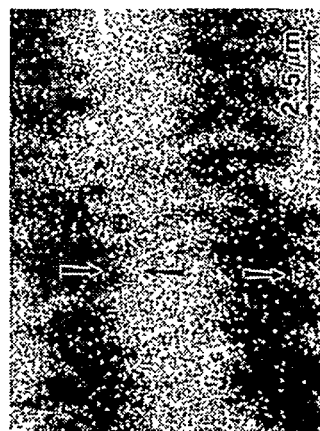


Figure 3. Examples of industrial and basic research that has been performed at LANSCE.

Why Does Livermore Need LANSCE?

*R. Fortner, Associate Director, Physics and Space Technology,
Lawrence Livermore National Laboratory*

Introduction

Five years ago, I was the associate director of the nuclear test program, so I have a really close view of the role of the nuclear testing in the weapons program. My perceptions are strongly driven by the fact that we have lost testing and what that really means. I want to explain to you why I think we really need a science-based stockpile stewardship program and what the issues are in terms of having lost nuclear testing.

When we think about this program, we really think that nuclear deterrents are part of a national policy and nuclear deterrents must therefore be credible, in Vic's words, competent. Now, nuclear weapons in the stockpile work as designed. The issue of science-based stockpile stewardship is not to go and improve the designs, but we know that problems are occurring in the stockpile and more problems will occur. Sometimes these problems are in individual weapons, and sometimes they are in complete systems.

The Loss of Nuclear Testing

Nuclear testing was a very cost effective way of doing business because we could build a system, take it out, test it, and find out if it performed. However, we do not have a detailed understanding of nuclear weapons from these tests. Our understanding of the physical systems and the tools we have are fundamentally inadequate. We have a list of 10 experiments that we did in the last 5 years of nuclear testing for which we cannot explain the data today. In the past we did not go out and test whether a problem was a problem; we tested if a fix was actually a fix. Nuclear test data by itself is inadequate so computational tools will be extensively used. Science-based stockpile stewardship basically says let us develop and certify the computational tools through relevant experiments that evaluate if these prob-

lems in the stockpile are real problems and if we can fix them.

We have lost testing, and we cannot build one simple system that is going to replace nuclear testing. The problems that we have are very complex and we have to address them with many capabilities. Understanding what nuclear data we have is critical. We know in many cases that we have data, which are better than the data we currently use in our code, but the capacity of our computers right now is inadequate to put the best detailed physics into our computational tools. We need better computational capabilities.

We need better experiment facilities. We designed the experiment facilities that we had in the past in an era when we had nuclear testing. We know that these facilities are not the kinds of facilities we need when we do not have nuclear testing. We need a variety of tools, which include pulsed-power facilities, the National Ignition Facility (NIF), and many new facilities to understand and certify a weapon. Hydrodynamic facilities were also designed in an era when we had testing. Improving the hydrodynamic facilities is clearly something that has to be done to meet our needs. This is a description of an advanced hydro facility, the Dual-Axis Radiographic Hydrodynamic Test (DARHT) facility at Los Alamos.

Confidence in the stockpile is not going to be accomplished by one set of activities, but by a plethora of activities. In the past, we performed nuclear testing to look at how a nuclear weapon would perform. Nuclear weapons take a large amount of mass and generate an enormous amount of energy, from hundreds of kilotons to tons of nuclear energy, during a nuclear test. In the future, we can test only the beginning part of the spectrum. When nuclear energy is produced, we get into the regime of secondaries and will not have the ability to measure what is happening.

An approach to science-based stockpile stewardship is to reduce the amount of energy that we are going to produce and achieve instead of the energy densities of the materials (Figure 1). The goal is to take a small amount of material and achieve the same energy density that we did in a large amount of material during a nuclear test. In addition to achieving the kinds of conditions that occur in nuclear weapons, we want to be able to understand the processes that are going on. Most of our experiments in the past have been integral experiments in which many physical processes are taking place at one time. To do carefully crafted experiments, we need to understand a detailed piece of the physics problem so it can certify our computational tools. We need to understand the processes along this entire path, not just one thing in one location. Many different facilities are being proposed because not one particular tool solves all the problems.

Diagnostics are critical. If we are going to do experiments to understand the properties of what is going on, we need to be able to diagnose what is going on. We get a great boost in science because this program is focused on detailed understanding. It is not just how does a weapon in the stockpile work, but what are the

processes that take place in nuclear weapons, and do we understand them?

Livermore Needs LANSCE

Livermore really needs the Los Alamos Neutron Science Center (LANSCE). The NIF needs LANSCE. If you look at the issues that we are going to have at NIF, such as the dose rates that are produced, LANSCE is the only facility that we can identify now where we can study the kinds of damage that can occur. We are trying to understand the damage, which is dose-dependent damage, that can be produced in materials like the glass at NIF by performing experiments at LANSCE that look at the optical properties.

The critical issue of NIF is how many shots can we get. The activation of the target chamber determines the number of ignition shots that you can achieve. With the large number of people that want to come to NIF and do experiments, we have recognized that the demand on NIF for doing ignition shots is much larger than originally conceived. If we look at the nuclear physics data that we used to estimate the activation of the target chamber, we realize that nuclear physics is very

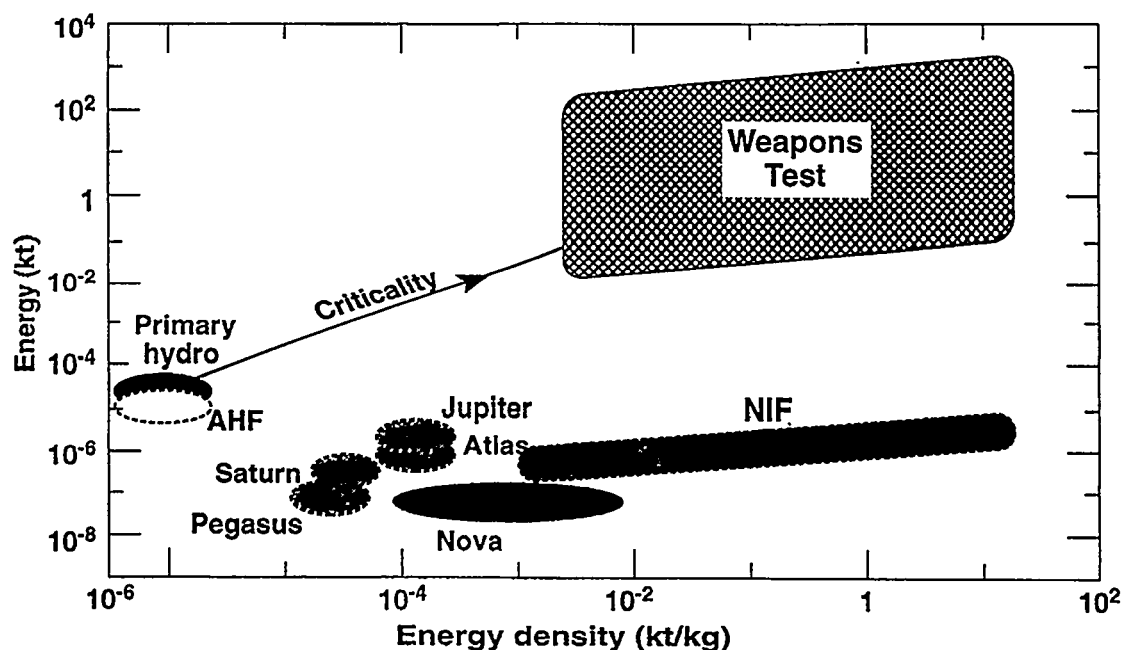


Figure 1. Science-based stockpile stewardship focuses on improving predictive capability by doing high-energy density experiments.

conservative. We use very large cross sections. We would like to know what the actual cross section is and if we can go back and more effectively use NIF by putting better nuclear physics into our estimates?

In the last 6 months, Livermore has looked at the accelerator production of tritium (APT). We started out as skeptics, and now we are believers that the project is on a sound foundation. We also believe that we can contribute to the project. If you look at the numbers, a 1% increase in the electrical efficiency of APT turns out to be a million dollars a year or 40 million dollars over the life of the accelerator. Also, if the yield of the target can be 30% higher than is currently estimated in terms of our nuclear physics understanding, we can save 150 million dollars over the cost of the accelerator. Understanding the details of the production of tritium is a critical area.

The thought of using high-energy neutrons to look inside materials is a very exciting prospect. We know that there will be applications. We want to understand just how far we can push those applications. All of this is tied to our understanding of basic sciences and nuclear physics and spills off in all these other areas.

This nuclear data can be very important in studying the radiation treatment of cells—the issues of radiation oncology. We use our Monte Carlo simulation to understand how we can produce damage in a tumor that might exist in a lung. Within the last few years, the medical community has talked to us about the issue of treating prostate cancer. In the past, the medical community treated prostate can-

cer from the front and the back because they thought that the energy loss in the hip would destroy our ability to put the energy into the tumor. We have convinced them this is not the case. Now they are looking at the possibility of treating tumors by doing radiation from four sides, which means that the collateral damage to the tissue surrounding the tumor could be much smaller and the actual dose rates to the tumor could be much higher. The medical community needs better cross sections and needs to understand these cross sections to much higher accuracy than currently exists.

Data on what happens to the actinides under high temperatures and high pressures does not exist. The importance of this data for understanding the equations of state of actinides as they occur in weapons is critical for stockpile stewardship. We are very excited about the possibility of looking at actinides under high temperatures and high pressures.

To predict the behavior of chemical explosives and their aging process involves an interrogation of chemical explosives and understanding the relationship of the phonon spectrum and the vibron spectrum. LANSCE has really high potential to look at structures and shock materials in the area of chemical explosives.

We are talking about the fundamental understanding of properties that are problematic, which is another talk in itself. When we get to the fundamental understanding of problematic materials, we find that this understanding has tremendous spinoff into the scientific community.

Lab Interdependencies and the Advanced Design and Production Technologies (ADaPT) Initiative

*D. Hayes, Director, Defense Programs Capabilities,
Sandia National Laboratories*

Introduction

I am delighted to be here today. I was left with a very strong impression this morning about the large degree of integration that has been achieved in the science-based stockpile stewardship program in the last year. When Vic Reis convened this program last February, many of you same people from Energy Research, Defense Programs, and the external community were there. We talked about areas of investments: in credible capability and industrial interaction, the impact on the research community, and so on. The product was the published quality function deployment chart. The activities on the chart were important, but they did not have coherence. In listening to the presentations this morning, particularly the last four, I hear a high degree of coherence and integration, which is very pleasing.

Four Initiatives in the Stockpile Stewardship Program

There are four initiatives in our stockpile stewardship program. There is the accelerator production of tritium (APT), National Ignition Facility (NIF), scientific computing initiative (ASCI), and the Advanced Design and Production Technologies (ADaPT) Initiative. ADaPT is a new acronym; the old name was factory of the future, which appeared as one of the pillars that John Immele discussed.

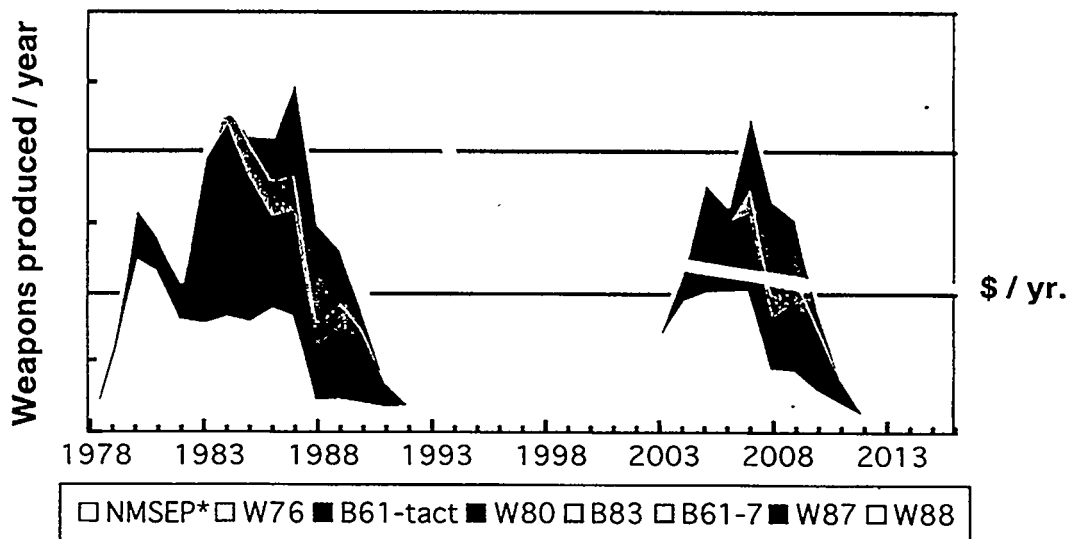
ADaPT really concerns itself with developing the technologies and the scientific underpinnings that can achieve actual delivery of a product to the stockpile. Of the four initiatives, I like to think of it as the one that is "closest to the wrenches." On the other hand, we know from past experience that we cannot execute this product realization unless we build our program quite robustly and integrate it quite deeply into our tech base. Within the program elements of ADaPT, you will find a

very deep scientific root, which really characterizes our approach.

Vic showed this viewgraph (Figure 1). Ev Beckner said that this was the most important viewgraph that Sandia had ever made, at least in the last year. I would agree. I want to use it not to repeat what Vic had to say, but just to make a couple of additional points. If you recall, the viewgraph represents the number of weapons that were produced per year versus the year they entered the nuclear weapons stockpile. For instance, the W-88 is the warhead that goes in the Trident submarines. These warheads were built in a short period of time, and we had to have a production capacity that was quite large. If we look at the design lifetime of these weapons and determine when they have to be replaced, rebuilt, or recertified, we find that they clump at a level that requires a quite large capacity. On the other hand, we are trying to build a production complex, which is focused in the laboratories, that has a very much smaller capacity. To cope, we can *start earlier* or *try to extend the certified lifetime*, which means that the lab directors are going to have to certify a stockpile in the future without the benefit of underground testing.

Another important point is that in this intervening time between when these weapons were first designed and manufactured and in the future when something has to be done, we have a quiescence period. We run the risk of losing our experience base, and we have to decide whether or not we are going to have the experience reside in people or if we are going to somehow capture it some other way.

All of these factors are the drivers for the ADaPT Initiative. If you look at the defining documents from the military, what you find is that ADaPT is the vehicle that does what the military prioritizes: the ability to replace, to



* DOE flight and lab tests

Figure 1. The weapon rebuild profile is the driver for the ADaPT initiative. (Printed from best available copy.)

requalify, and to recertify the weapons in the enduring stockpile.

ADaPT has three facets. The first facet is to assure that we have the capability to make products. The second facet is that we have a confidence in the stockpile that comes from the certification. The third facet is to ensure that we have a robust people base capability.

The Program Elements of the ADaPT Initiative

I will discuss some of the ADaPT Initiative elements including advanced materials and processing, virtual manufacturing, information and communication, and modeling and simulation. Advanced materials and processing is represented, for instance, by a precision plutonium casting facility. It may be in the future that we have to directly cast pits to final shape. This requires a whole new set of technologies, including materials, metallurgical casting, and so on. If we have to remanufacture pits, we will do it in a way that produces the smallest amount of waste.

Virtual manufacturing means that we do not want to design a facility and find out that it is not right. We are going to need something that is robust to change and try different capa-

bilities in the computational environment and virtual manufacturing before we actually commit the facilities, hardware, robotics, and so on.

Information and communication will help us to reduce the design cycle time from concept to first product delivery. We are trying to do things concurrently. We are connecting people who have various functions in design and producing prototypes, so they have access to the right kinds of information, particularly very robust models that we build for modeling and simulation, environmental concerns, and other concerns. People will have an electronic environment in which they can do the design and have access to other key players and key information that they need to do their job.

We have heard a lot about the modeling and simulation. This computational environment will draw very heavily on ASCI, the accelerated scientific computing initiative, because many of the models are quite complex and require large codes and intelligent ways of programming in the massively parallel environment. I want to highlight this program element because there is a companion set of issues that have not to do with just the design process, but the design and validation process. We are changing the way we actually do design

and execute production. At one extreme, we say that we can define requirements, do a design, produce something with periodic tests of prototypes. We find that we are going to have to rely more and more not on testing the prototypes or the products, but validating the models that are used to design that product. If we invest this way, we will have the confidence that these models are giving us the right answer. We will have only selected tests or prototypes to validate our analysis tools. We will be able to cycle information back into the design considerations. Of course, in all of the laboratories we have always had this balance between testing the product and testing the models. What I see is a shift in emphasis toward testing the models and less testing the design. In the case of the nuclear package itself, we cannot do any proof tests at all because underground testing is not allowed.

The following topics highlight a safety theme, not a performance theme. We see that in the case of extreme environments produced by an airplane crash that we are going to produce undesirable environments. The public is going to demand that we certify the safety of these systems to a higher level than we have ever done before. I believe that we are going to rely more on our computational tools not only to model the total system, which is being insulted here, but also the individual safety components. We have to add computers to our suite of tools that we use to certify weapons systems and subsystems. We have the high-

performance computing and validated design tools and a suite of test facilities, radiation facilities, select environmental facilities, and a large category of other experiment laboratory facilities. One is our aerodynamics facility, but also included are the Dual-Axis Radiographic Hydrodynamics Test (DARHT) facility for primaries or NIF for the verification models.

Spallation Neutrons are Advantageous to Research

I have one example that talks about the acceleration of ions (Figure 2). We must ensure that as we build this capability we do not keep duplicative capabilities because we do not want expensive redundancy in the system. We see that the radio-frequency systems, like the Los Alamos Meson Physics Facility, will be very complementary to those pulsed-power systems, which have the ability to accelerate a very much larger number of ions with a smaller ion energy. These ions produce dramatically different neutron spectrum when you convert them. In the case of spallation neutrons, we get energies that are almost 2 decades above what is achieved by tunable ion kinetic energy impulse power system.

In summary, the ADaPT Initiative should assure us that we have a robust product realization capability, we have a way to express a confidence in the stockpile, and we maintain a skilled work force especially through this transition period. It will operate in a downsized

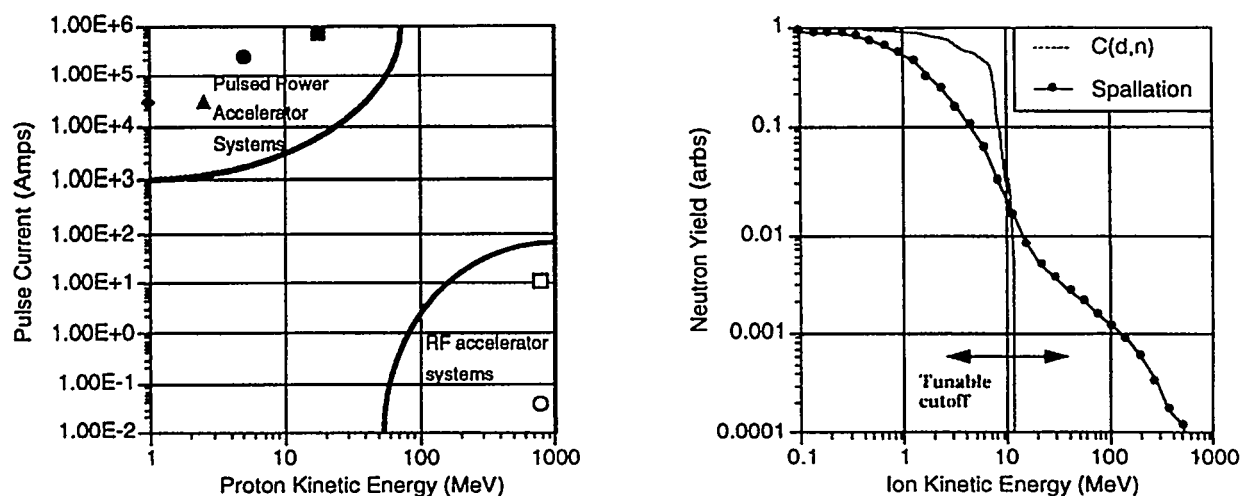


Figure 2. Pulsed-power and radio-frequency systems provide complementary capabilities.

production complex, of which we can already see evidence by the plant closings. We are going to minimize our duplication of capabili-

ties, and the lower operating cost is going to be necessary considering our lower budget considerations.

TECHNICAL SESSIONS

*Workshop on Defense, Basic, and Industrial Research
at the Los Alamos Neutron Science Center*

Neutrons for Technology and Science

G. Aeppli, AT&T Bell Laboratories

Abstract

We reviewed recent work using neutrons generated at nuclear reactors and accelerator-based spallation sources. Provided that large new sources become available, neutron beams will continue to have as great an impact on technology and science as in the past.

Introduction¹

Even after a century of unprecedented improvement in living standards because of technology, there are still many needs that only further applications of science can meet. These needs are in areas ranging from medicine to transportation. They include cures for AIDS and Alzheimer's disease, improved productivity in health care delivery, electric vehicles, supersonic airliners, loss-less electric power transmission, reliable nuclear waste disposal, nontoxic solvents, procedures for oil spill cleanup, and affordable low-power wireless communications with global coverage. While national and corporate governments can affect economic life by redistributing wealth, net wealth increases only via technological progress, namely progress on meeting needs of the type just listed.

In addition to needs for specific items which will increase the comfort and safety of human existence, there are cultural needs which have no clear material origins. Most fundamentally, there is the need to discuss, if not to answer, the questions of how the universe began and how long it will last and whether quantum mechanics and Einstein's theory of relativity are sufficient to describe the physical universe. The enormous success of Hawking's book, *A Brief History of Time*, attests to the size of the nonspecialist audience taking an interest in

such questions. Beyond its philosophical appeal, basic science has a history of leading to unexpected breakthroughs which are missed by programs to develop obvious technologies.

After a brief survey of neutron properties and sources, the present article describes how research at neutron facilities has recently met both technological and cultural needs, and argues how it will continue to do so in the future.

Neutrons and Neutron Sources²

The neutron is a spin 1/2 particle with no electrical charge and the mass of the proton. As produced at facilities dedicated to materials research, neutron wavelengths are comparable to interatomic spacings, and energies are comparable to those of vibrations in solids and liquids. The neutron interacts almost exclusively with magnetic fields and nuclei. Both couplings are relatively weak and known with great accuracy, implying that neutrons scatter from matter according to a law which is simpler and more precisely specified than for any other probe (e.g., photons and electrons).

Most neutron scattering experiments to date have been carried out at nuclear reactors ranging in power up to 85 MW, but more typically with powers between 10 and 30 MW. For comparison, commercial power reactors, with much larger core volumes, have ratings of order 1 GW. The moderator blankets surrounding the fuel elements determine the neutron energy and wavelength distribution. The primary moderators for research reactors are generally liquid D₂O, held near room temperature, yielding a Maxwellian neutron spectrum with a peak near 25 meV \equiv 300 K. Secondary moderators held at lower or higher temperatures can shift the spectrum to lower and

¹ Published in © OECD, 1994, "Neutrons for Technology and Science" in *Neutrons Beams and Synchrotron Radiation Sources, Megascience Forum*. Reproduced by permission of the OECD.

² This discussion is largely excerpted from that by G. Aeppli et al. in *Lecture Notes for E. Fermi Summer School*, Varenna (1992), to be published by the Italian Physical Society.

higher energies, respectively. The most common secondary moderator contains hypercritical hydrogen or liquid deuterium held at 25 to 35 K and constitutes the "cold source" at most European reactors. For the study of high-energy (≥ 50 -meV) excitations or phenomena at high momenta, the neutrons can be re-thermalized by a block of graphite heated to 2400 K by the γ rays from the reactor core. This is a "hot source," and is much less common than cold sources. Figure 1 shows the arrangement of core, moderator, and beam extraction tubes at the Institut Laue-Langevin (ILL) in Grenoble, France, while Figure 2 shows some source spectra at the same facility. The small core size (roughly 50 cm in diameter) and concomitant high-power density makes the ILL, along with the Oak Ridge, Brookhaven, and the proposed U.S. Advanced Neutron Source (ANS) reactors, unique as high-flux neutron sources compared with both commercial and other research reactors.

An exciting recent development has been the construction of accelerator-based spallation sources where neutrons are produced not in a steady-state nuclear reaction, but by bombarding a target containing heavy elements such as Ta or U with energetic ($E \sim 1$ -GeV) protons. The neutrons are subsequently cooled (via multiple scattering) in small (typically $10 \times 10 \times 5$ cm³) moderators tailored for the experiments they serve in much the same way that the insertion devices in third generation synchrotrons are designed for specific instruments. The advantages of this source type include its pulsed nature, yielding great improvements both in spectrometer efficiency and background rates, an incident neutron spectrum extending to high energies, good intrinsic resolution, and obvious intrinsic safety (the source is shut down when the proton beam is off). Figure 3 shows the layout of ISIS (UK), the world's most powerful source of this type. Its time-averaged neutron flux is roughly 1/30 of that at the ILL, but its

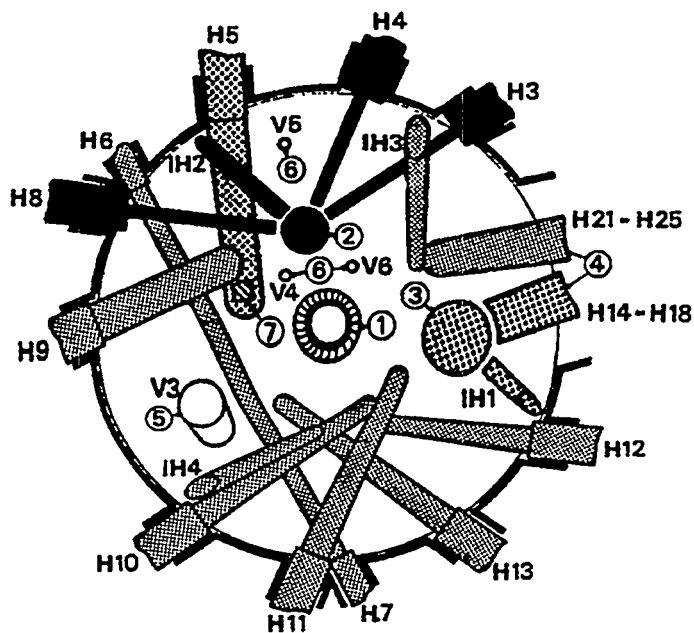


Figure 1. Configuration of ILL reactor in Grenoble, France. Numbers 1, 2, 3 and 7 denote core, hot source, vertical cold source, and horizontal cold source, respectively. Numbers preceded by 'H' label neutron beam tubes. From Guide to Neutron Research Facilities at the ILL (Grenoble, 1988) by H. Blank and B. Maier.

peak flux is larger, particularly at high energies; a new European spallation source (ESS) with the same average flux as the ILL and a peak flux 40 times larger is currently under consideration.

Technology

Technological needs are needs for materials and algorithms. Neutrons, with wavelength and energy definition tunable through all scales relevant for the physical behavior of solids and liquids, and a well-defined and simple scattering cross section, are an ideal probe of materials. Recent years have seen growth in studies of polymers, biological materials, and actual engineering components. For example, small-angle scattering experiments have revealed the many ordered bulk structures, correlated with function, which diblock copolymers can achieve. At the same time, reflectometry has elucidated the different surface

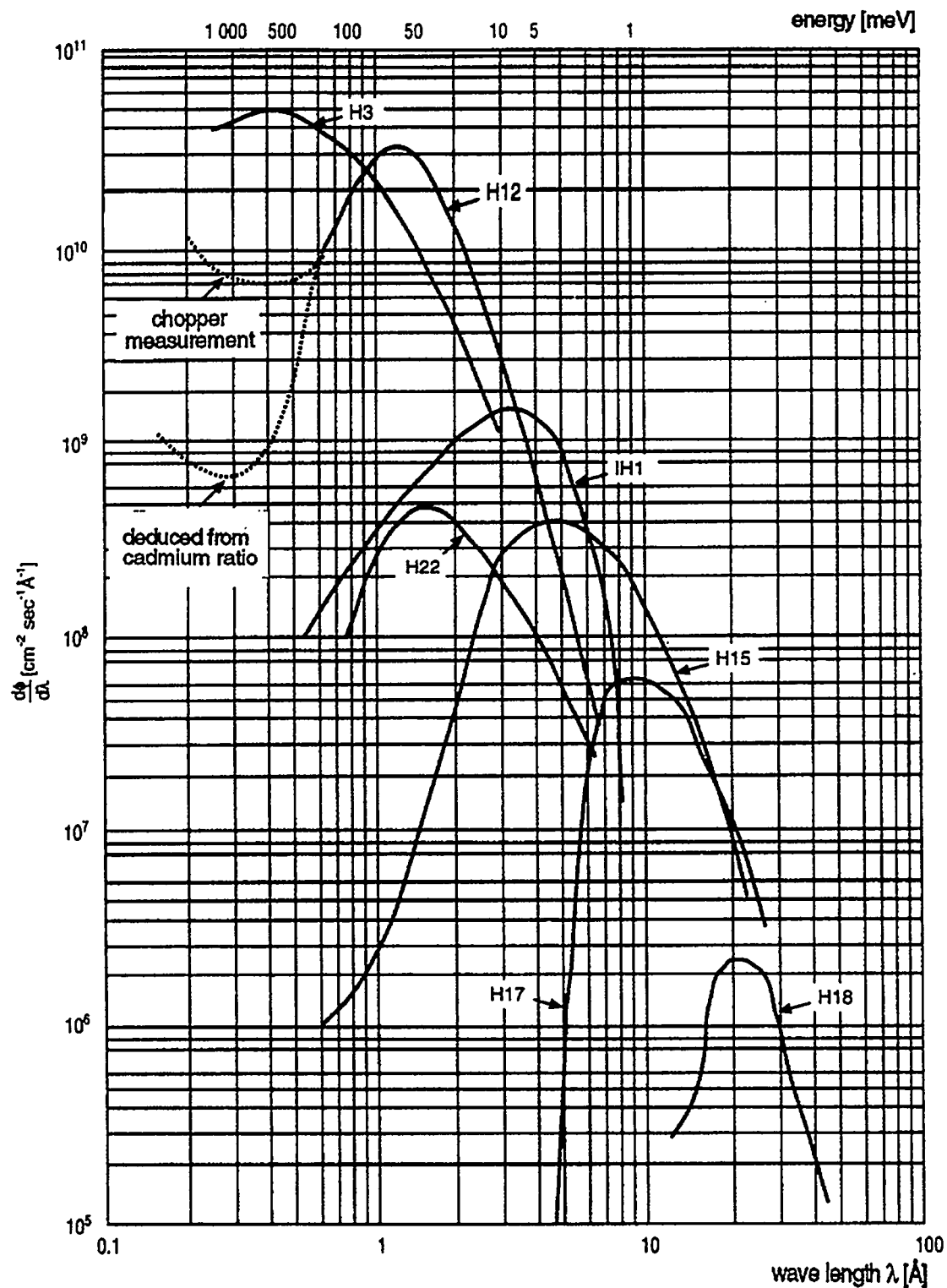


Figure 2. Spectra of neutrons at various neutron beam tubes of ILL reactor. Designation of beam tubes is as in Figure 1. From Guide to Neutron Research Facilities at the ILL (Grenoble, 1988) by H. Blank and B. Maier.

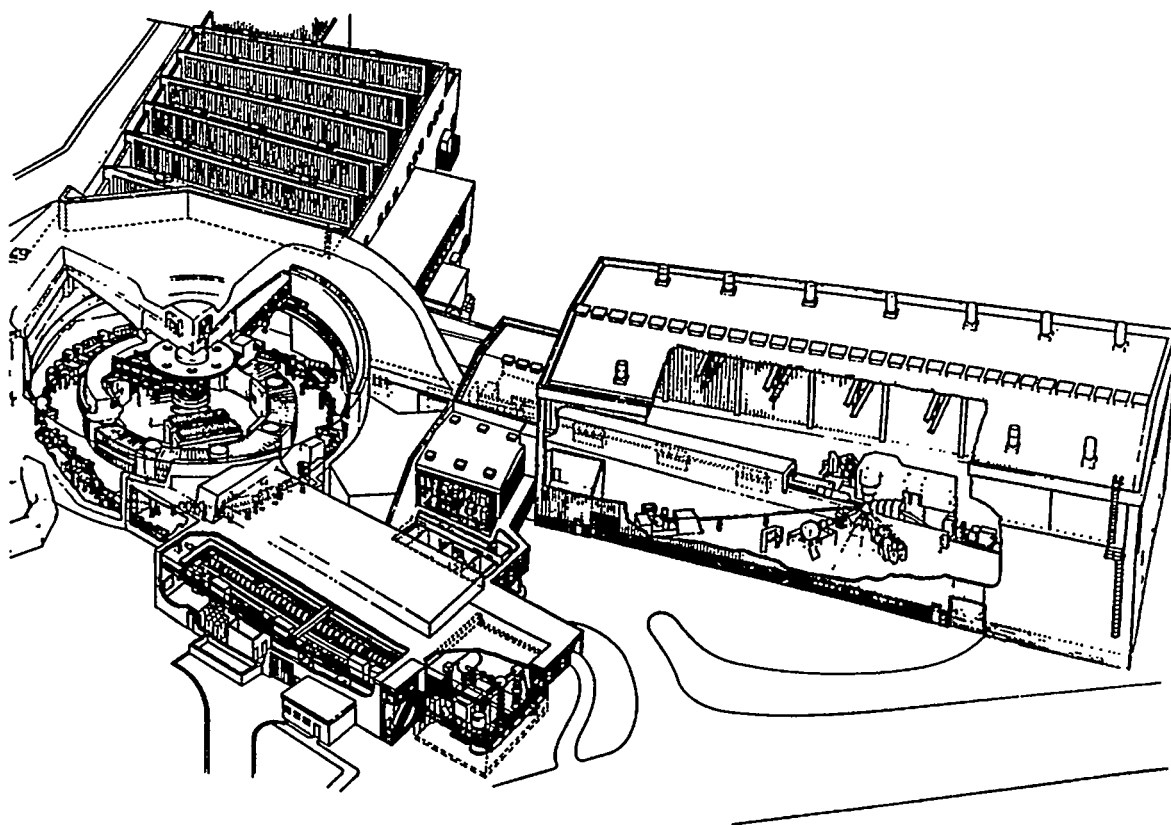


Figure 3. Layout of ISIS spallation source at the Rutherford Appleton Laboratory (RAL), UK. Protons proceed from injector at lower left to synchrotron at left and then to neutron producing U (or Ta) target in beam hall at right. Figure provided by A. Taylor (RAL).

configurations for such polymers. Figure 4 shows how neutron reflection profiles are an excellent diagnostic for determining whether the polymers are in an entangled "mushroom" or an unentangled "brush" state: the state determines their utility in applications such as oil recovery and colloid stabilization. Moving from polymers to hardware of the most traditional kind, neutrons have been used to measure strain distributions in an increasing variety of situations, ranging from welds to rotating jet turbines. Figure 5 illustrates the technique, which exploits the penetrating power of neutrons, and therefore makes it possible to perform *in situ* validations of algorithms routinely used by engineers to calculate strains as well as to understand component failures.

There has also been considerable progress in more traditional materials research, namely work to determine the structure and to understand the properties of the many new com-

pounds created yearly. Among the most dramatic to be discovered recently are the hard mixed iron rare-earth magnets increasingly deployed in small motors such as those in automobiles. Not surprisingly, neutrons, with their sensitivity to magnetic order and dynamics, are currently being used to examine these materials with a view toward gaining a microscopic theory to further enhance their properties. Other exciting new compounds are those based on the carbon-fullerenes whose crystal structures and rotational dynamics were established very shortly after their discovery by neutron scattering. Recent developments in sources and instruments now permit collection of ultra-high resolution powder diffraction patterns such as that shown in Figure 6, taken at ISIS for a fullerene. The intensities of the extraordinary number of resolved peaks specify the structure of the material, which has 480 atoms per unit cell, with unprecedented detail and precision. Unfortunately, space does

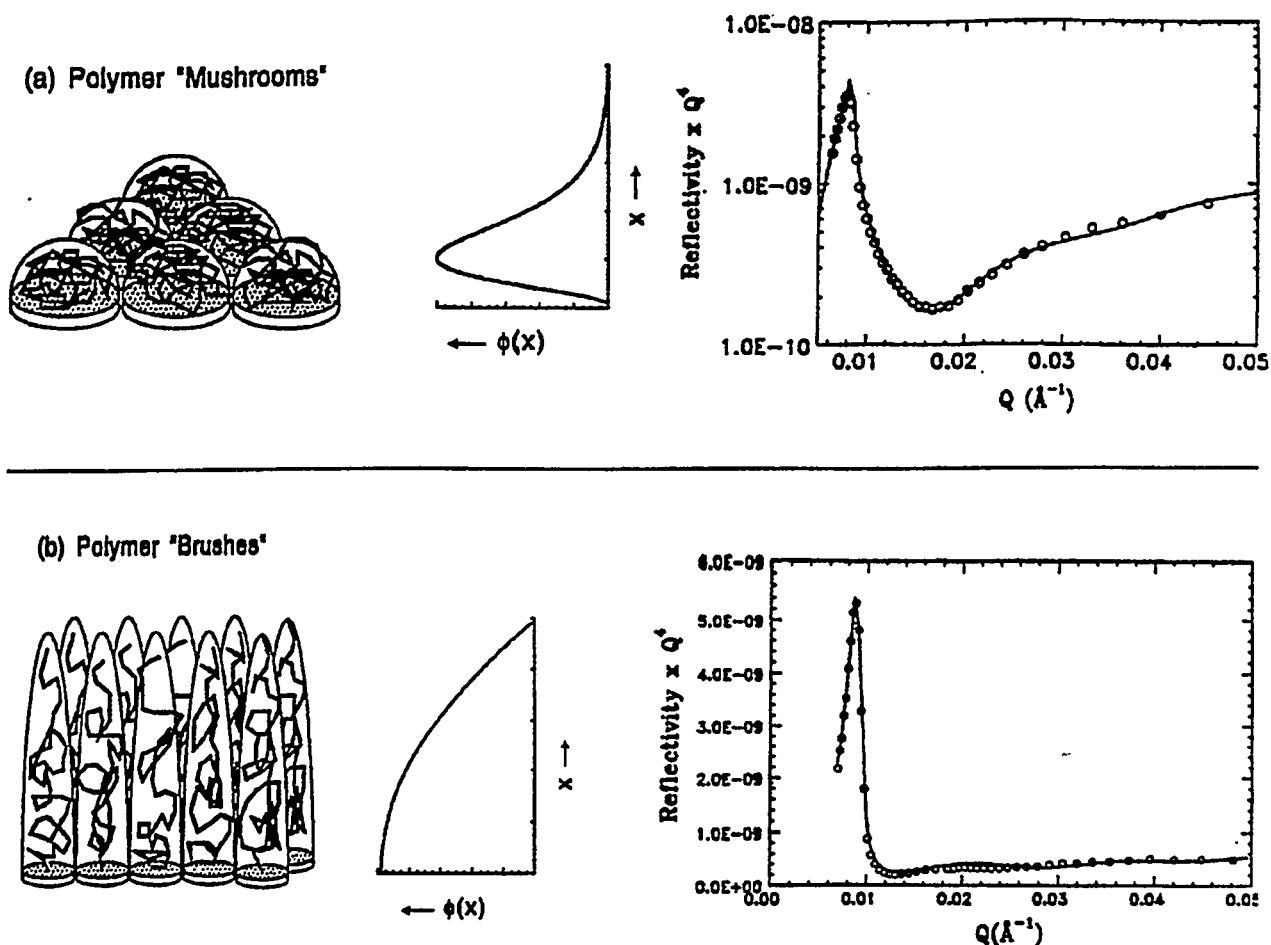


Figure 4. Neutron reflectometry from adsorbed diblock copolymers. The experiments, which measure the scattering near grazing incidence, provide density profiles (middle frames) perpendicular to the surfaces on which the copolymers reside. The wave number Q is measured in \AA^{-1} ; $1 \text{ \AA}^{-1} = 10^8 \text{ cm}^{-1}$. Figure provided by R. Pynn, Los Alamos Neutron Science Center (LANSCE, U.S.).

not permit mention let alone discussion of all of the useful materials being examined with neutrons. However, to give the reader a sense for the huge variety of studies being pursued, Figure 7 shows a page from a random listing of neutron scattering papers published in 1992. We see that there is work in areas as disparate as molecular biology and shape memory alloys, and that each experiment uses a unique capability of neutrons to extract essential information not accessible by any other probe.

Arguably the most important event in the world of materials of the last decade was the discovery of the high- T_c superconductors. We discuss these systems in greater detail than the others mentioned above both because they are more familiar to the author and also because neutrons have provided fundamental informa-

tion on very different aspects of the compounds. We introduce the subject by recalling that superconducting materials, with their ability to exclude magnetic fields and conduct electricity with zero losses, have always held great technological promise. Indeed, superconducting magnets are now routinely used in applications ranging from particle acceleration to magnetic resonance imaging (MRI) at hospitals. Superconducting quantum interference devices (SQUIDs) are at the heart of ultrafast oscilloscopes and sensitive magnetometers employed in fields as diverse as oil prospecting and brain science. While the manufacture of products based on superconductors constitutes a sizable industry, it would be far larger if materials superconducting above the boiling point of cheaply generated liquid nitrogen were

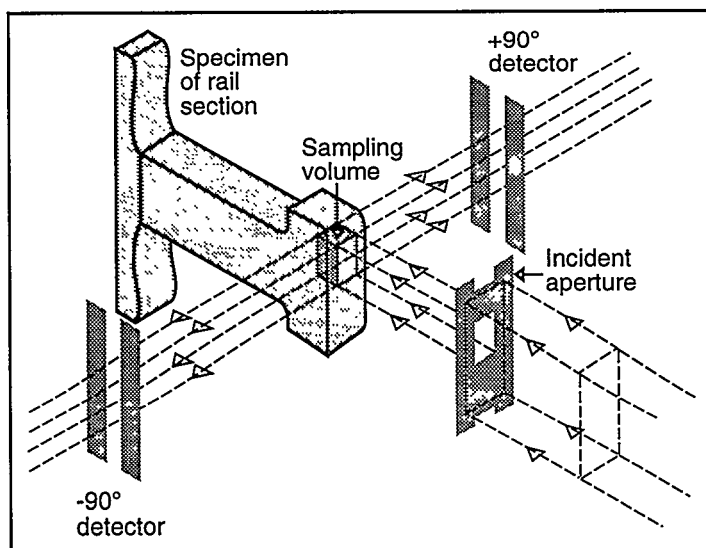


Figure 5. Neutron strain measurements. Incoming neutrons pass through incident aperture and are scattered at right angles. A three-dimensional strain map is constructed by scanning the volume defined by the intersection of ingoing and outgoing beams. Because of the penetrating power of neutrons, virtually any engineering component can be examined in this way. Figure provided by R. Pynn (LANSCE, U.S.).

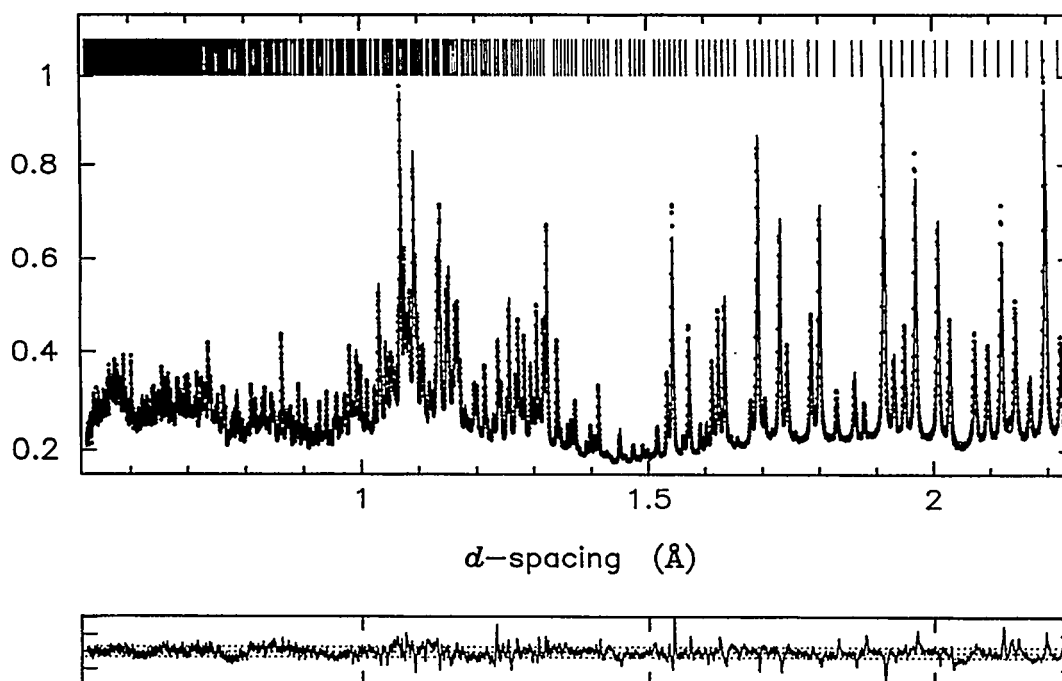


Figure 6. Ultrahigh-resolution powder diffraction pattern collected for C₆₀ (fullerene) using pulsed spallation source ISIS in UK. Because of the large number of resolved peaks, the atomic positions and thermal parameters can be determined with unprecedented precision. Top frame shows data (circles) and fit to data (line) while bottom frame shows the goodness of fit, as measured by the difference between the data and the fit. Figure provided by W. David (RAL).

Authors: Mayer-HM Steiner-M Stusser-N Weinfurter-H
Dorner-B Lindgard-PA Clausen-KN Hock-S
Verhoef-R

Title: Inelastic Neutron-Scattering Measurements on
Nd₂Fe₁₄B and Y₂Fe₁₄B Single-Crystals

Source: JOURNAL OF MAGNETISM AND MAGNETIC
MATERIALS
1992, Vol 104, Iss FEB, pp 1295-1297

Authors: Planes-A Manosa-L Vives-E Rodriguezcarvajal-J
Morin-M Guenin-G Macqueron-JL

Title: Neutron-Diffraction Study of Long-Range Atomic
Order in Cu-Zn-Al Shape Memory Alloys

Source: JOURNAL OF PHYSICS-CONDENSED MATTER
1992, Vol 4, Iss 2, pp 553-559

Authors: Wagner-W Boni-P Wiedenmann-A Petry-W

Title: Neutron-Scattering Study of Magnetic Correlations in
Nanostructured Fe

Source: PHYSICA B
1992, Vol 180, Iss JUN, pp 105-107

Authors: Langan-P Forsyth-VT Mahendrasingam-A Alexeev-D
Fuller-W Mason-SA

Title: A Neutron-Diffraction Study of the Distribution of
Water in the A-Form of the DNA Double Helix

Source: PHYSICA B
1992, Vol 180, Iss JUN, pp 759-761

Figure 7. A page from a computer-generated listing of neutron scattering papers published in 1992. Nd₂Fe₁₄B, in title of first paper in this list, belongs to the family of hard magnets mentioned in text.

available. A series of breakthroughs, beginning with a discovery at the IBM Zürich Laboratory in 1986 and 1987 yielded precisely such materials, namely layered oxides of copper.

The key questions about new materials are always the same:

1. Where are the atoms?
2. What are the electrons doing?
3. What happens under practical circumstances, i.e., when there are magnetic fields, electrical currents, and disorder?

Questions 1 through 3 were immediately asked about the cuprates, and have been, to a very

significant degree, answered by neutron scattering experiments whose success often depended on modern instrumentation which was just becoming available as the new superconductors were being synthesized. In particular, neutrons with their equal sensitivity to light and heavy atoms, provided the definitive crystal structures for all of the high-T_c materials, almost always within weeks of the discovery of new compounds. The crystal structures are invariably correlated with superconducting properties, sometimes in surprisingly simple ways. For example, mercury-based cuprates have the highest superconducting transition temperatures on record. Pressure has a very pronounced effect on the transition

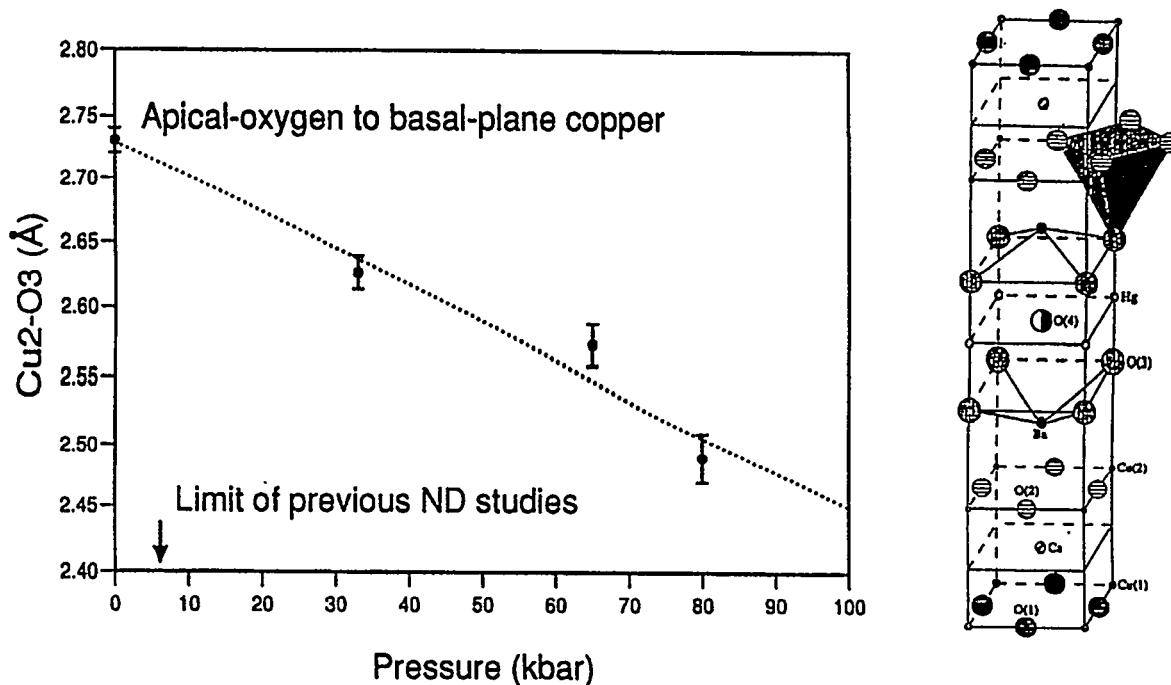


Figure 8. Pressure dependence of distance between apical oxygen and nearest copper atom, which is shortened by 0.25 \AA as the superconducting transition temperature rises from 132 K $\sim (-143^\circ\text{C})$. This material is the mercury-based high- T_c superconductor whose crystal structure is illustrated at right. The apical oxygen is at tip of inverted pyramid and directly opposite the copper atom (small filled sphere) at the center of pyramid base. The experiment was performed at ISIS. Figure provided by W. David (RAL).

temperature T_c of one such compound, $\text{HgBa}_2\text{Ca}_2\text{Cu}_2\text{O}_7$, raising it from 132 K (-141°C) for $P = 1 \text{ atm}$ to 155 K (-118°C) for $P = 200 \text{ kbar}$. Taking advantage of the penetrating power of neutrons, a group at ISIS was able to measure the atomic coordinates for a sample mounted in a high-pressure cell. Figure 8 shows the outcome of the experiment, namely that pressure affects primarily the oxygen at the apex of the pyramids (e.g., shaded object in right-hand part of figure) surrounding the copper atoms responsible for superconductivity and indeed moves it by the extraordinary distance of 0.25 \AA on imposition of 80 kbar .

Beyond providing the positions of the atoms constituting the high- T_c superconductors, neutrons have also provided images of the outer valence electrons which are paired as spin singlets to produce the superconducting wave function. They do so because they couple via the magnetic dipole interaction to the spin and orbital momentum of unfilled shells. Be-

cause singlets cannot scatter, conventional pairing will eliminate the scattering below the pairing energy. Thus, magnetic neutron scattering is an excellent technique for mapping the gap function of superconductors. It is also unique because its weakly perturbing nature guarantees that it is a bulk probe with a simple cross section and because the neutron wavelength and frequency is well matched to the distances and energies relevant for high- T_c superconductivity. Figure 9 shows electronic scattering as a function of the two-dimensional wave numbers associated with the nearly square CuO_2 planes, which are the fundamental building blocks of all high- T_c materials. In this case, the host for the CuO_2 planes is $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$, which is among the simplest of the high- T_c materials. Four peaks dominate the normal state data (Figures 9a and 9b), and the peak positions provide precise values for certain dimensions of the Fermi sea wherein the charge carriers responsible for metallic conduction and, ultimately, superconductivity reside. These dimensions are strongly compo-

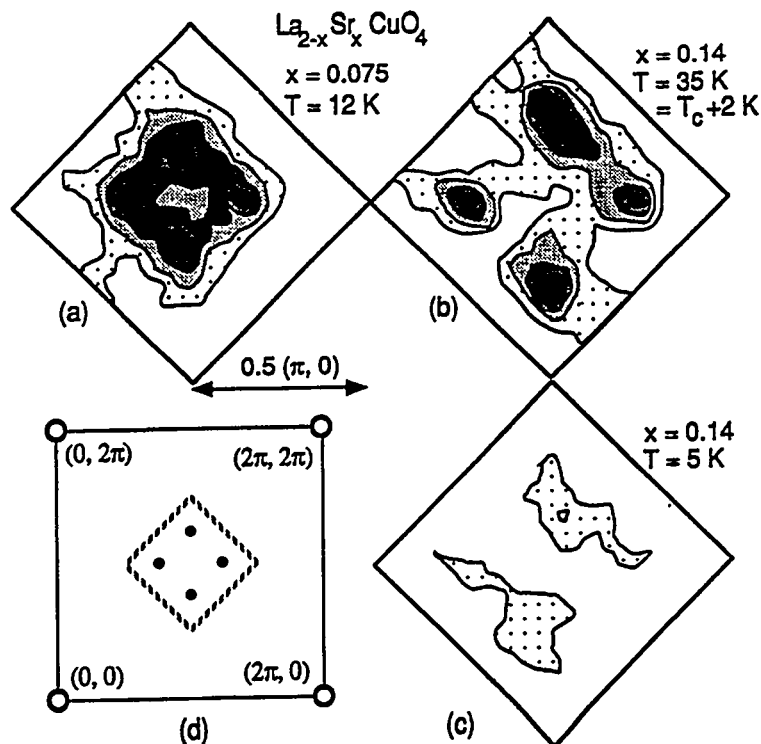


Figure 9. Maps of electronic correlations in $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$ for superconducting ($x = 0.14$) and nonsuperconducting samples ($x = 0.075$). The hatched diamond in frame (d) shows the region of probed wave numbers relative to the Bragg peak locations. For $x = 0.14$ (frames b and c), the signal essentially disappears on cooling through the superconducting transition temperature because the carriers pair to form spin singlets which cannot scatter neutrons. Data were collected at Risø DR3 reactor (DK). Figure provided by S. M. Hayden (Bristol, UK).

sition-dependent, as can be deduced from comparison of Figures 9a and 9b, which show the change in peak positions between nonsuperconducting $x = 0.075$ and superconducting $x = 0.14$ samples. Finally, comparison of Figures 9b and 9c shows that superconductivity, brought about by cooling from 35 to 5 K, largely eliminates the scattering peaks, and hence the Fermi surface of $\text{La}_{1.86}\text{Sr}_{0.14}\text{CuO}_4$. While other techniques yield individual parameters whose temperature dependence is consistent with singlet formation in superconductors, the data here represent the first microscopic image of spin pairing in any superconductor. Even though this is a very recent application of neutron scattering, such images have already been used to determine the detailed momentum dependence of the pair wave function Ψ in $\text{La}_{1.86}\text{Sr}_{0.14}\text{CuO}_4$. The resulting knowledge of Ψ allows many of the unusual

bulk properties of high- T_c superconductors to be explained and may eventually lead to their improvement for technical applications.

For the high- T_c materials to be useful, it is extremely important that they be able to carry substantial currents, especially in magnetic fields. Figure 10 shows early data which indicated that the copper oxides may not meet this requirement. The electrical resistivity of a particular cuprate with the quite high critical temperature of 90 K is compared with that of elemental copper, and for the relatively modest magnetic field of one kilogauss, the resistivity—and hence power dissipation—of the latter is lower for temperatures above 45 K. To engineer a truly useful high- T_c superconductor, it is obviously important to understand the mechanism for the large dissipation so far below the superconducting transition tempera-

ture. For conventional (low- T_c) superconductors, magnetic fields penetrate in an inhomogeneous manner, as defined by flux lines arranged on a regular and usually hexagonal lattice. The flux lines are usually immobile, being pinned by impurities. Because the flux lines dissipate power only when they move, the resistivity of most conventional superconductors in fields is indistinguishable from zero. Neutron diffraction, with its sensitivity to magnetic field inhomogeneities, provided the first microscopic evidence for flux line lattices in conventional superconductors. It should therefore come as no surprise that it has played a major role, especially at higher fields where no other techniques can image flux lines, in accounting for the large dissipation in the high- T_c materials. In particular, as do ordinary crystal lattices, the flux line lattice diffracts neutrons, and when the crystal or flux lattice melts, the diffraction peaks disappear. The frame on the left of Figure 11 demonstrates that the diffraction intensity vanishes, and hence that the flux lattice melts, at temperatures well below T_c , while the frame on the right shows the phase diagram for interacting vortices in the bismuth-based copper oxide superconductor in question. The vortex density is proportional to the applied magnetic field B . The neutron experiments are important because they provide microscopic evidence that, in analogy with what occurs for conventional materials whose fundamental constituents are molecules, flow will be both possible and dissipative when the vortices are in their molten state (right hand side of phase boundary in Figure 11).

Culture—Basic Science

All human societies have had cosmologies, that is theories about the beginning and potential end of the universe and about the meaning of things, such as stars, which we see but cannot visit. Modern cosmology is a very active area of scientific research, especially because it is very often related to fundamental questions in particle physics. Neutron research has been

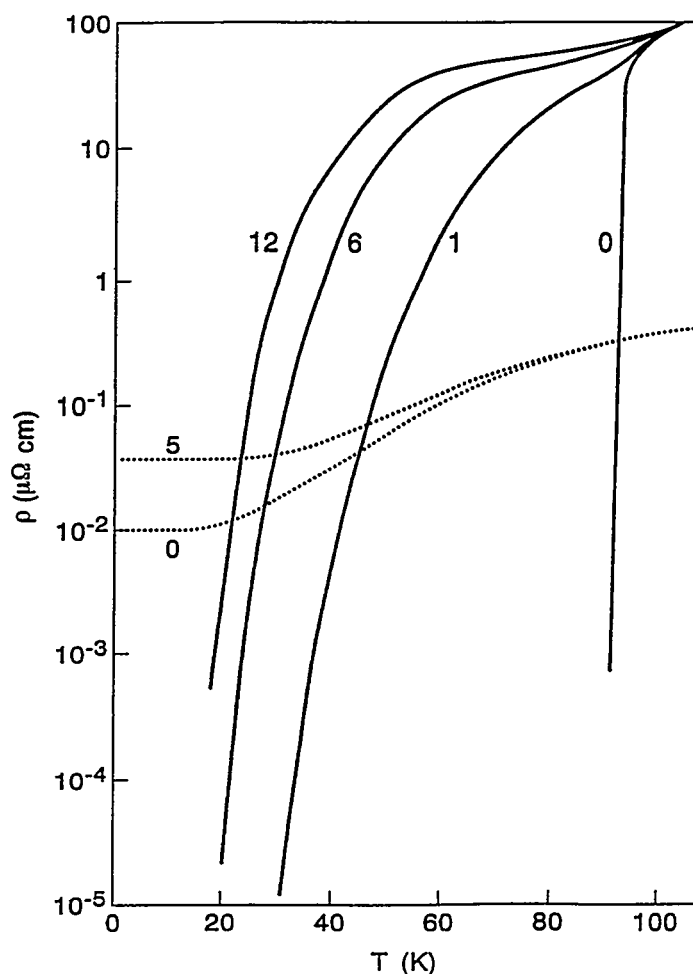


Figure 10. Temperature-dependent resistivity of high- T_c superconductor (solid lines) and elemental copper (dashed lines) in external magnetic fields denominated in kilogauss. Figure provided by D. J. Bishop (AT&T Bell Laboratories, U.S.).

able to play a role in this exciting field via measurements to place an upper bound on the neutron electric dipole moment and precision determinations of the neutron lifetime. The two experiments have implications for CP violation and baryon number density, which in turn are important in answers to the key questions of why the known universe consists of matter and not antimatter, and whether there is invisible, nonbaryonic ("dark") matter. Figure 12 illustrates how the limits on the neutron electric dipole moment have been reduced by six orders of magnitude over the last three decades, and how this reduction has restricted possible theories of elementary particles. A further reduction, which is relatively small on the scale of the reduction already achieved,

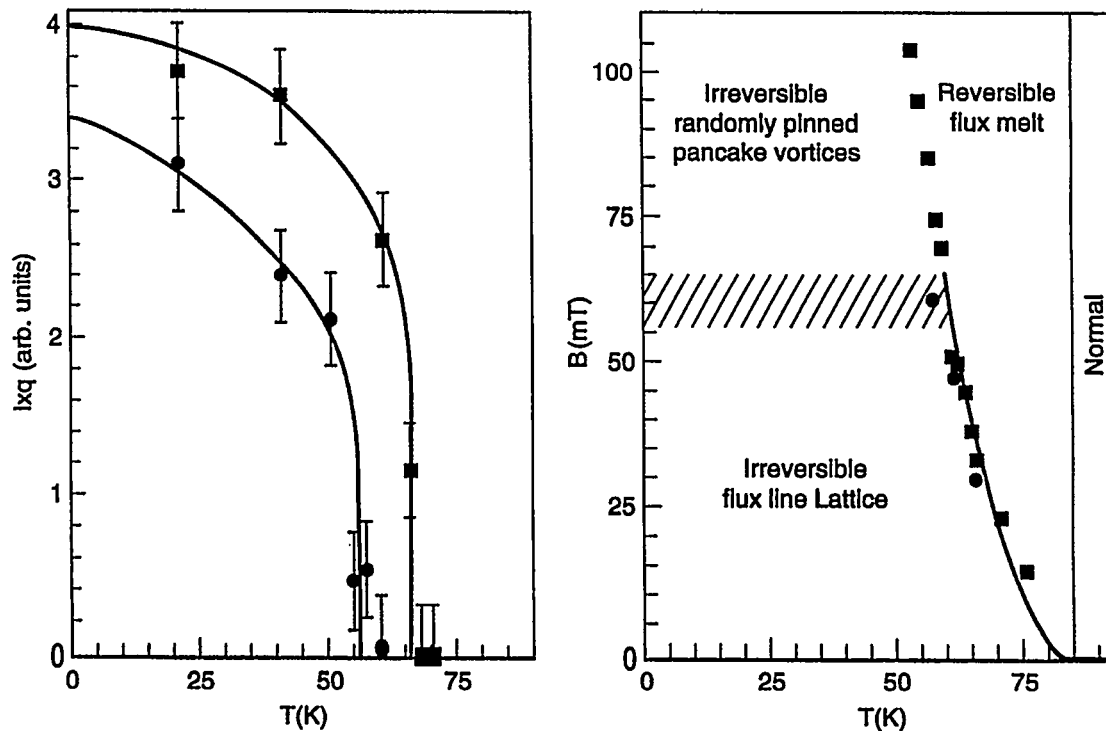


Figure 11. Left: Temperature-dependent neutron diffraction intensity which monitors the melting of the flux (magnetic vortex) lattice in a bismuth-based copper oxide high- T_c superconductor. Data are for 30 mT = 300 gauss (squares) and 60 mT = 600 gauss (circles). Right: Flux lattice-flux liquid phase diagram. Experiments were performed at Risø DR3 (DK) reactor. Figures provided by H. A. Mook (Oak Ridge, U.S.) and T. Forgan (Birmingham, UK).

will eliminate many currently popular models, namely supersymmetric (SS) theories, grand unified theories (GUT) which incorporate the observed baryon asymmetry, and left-right (LR) symmetric models.

Apart from cosmology, a topic of perennial interest (at least in this century) concerns the validity of quantum mechanics. On this subject, there have been precise tests of the validity of Schrödinger's equation for neutrons, as well as interferometric investigations of their wave-like nature. A particularly interesting recent experiment demonstrated the Aharonov-Casher effect, where the phase appearing in the neutron wave function is affected by a potential which imparts no classical force on the neutron. Thus, quantum mechanics, even for a simple uncharged particle such as the neutron, has consequences more profound than those suggested by wave-particle duality.

Also in the realm of basic science are the quantum fluids, ^3He and ^4He , as well as quan-

tum magnetism. The role of the neutron in investigations of these topics is well-established and far from exhausted. Probably the most exciting recent result is the verification of the Haldane conjecture, namely that a one-dimensional chain of antiferromagnetically coupled integer spins displays the structure function of a quantum liquid: the magnetic correlations are only of short range and there is a sharp gap to magnetic excitations above the singlet ground state. This is a very surprising result given that *half-integer* spin chains are nearly ordered in the sense of possessing infinite magnetic coherence lengths. Without neutron scattering, the Haldane conjecture, one of few nontrivial predictions of modern solid-state theory, would not have been verified.

The Future

There is no shortage of problems in technology and science which neutrons can help to solve in the future. As indicated in the introduction, there are many unfilled technological

needs which invariably entail needs for new materials or better understanding of known substances. The variety of materials explored with neutrons will continue to expand, especially to include more systems of biological interest and engineering components close to their end-use condition.

In addition to applying existing techniques to a larger variety of materials, new instruments such as RITA at the Risø (Denmark) DR3 reactor and MAPS at the ISIS pulsed spallation source will increase the efficiency of certain experiments by as much as two orders of magnitude, allowing the investigation of correspondingly weaker signals and smaller samples. Also, while the last decade has been the decade of the cold source in that it has witnessed an explosion in the use of long wavelength neutrons produced at such sources, the next decade will see not only further developments in this area but also an increased exploitation of the epithermal neutrons naturally produced at spallation sources and available from hot sources installed at reactors. Such neutrons will access excitations with energies in the midinfrared range so central to chemistry and solid-state science. The big advantage of the neutron technique, here, as always, is its well-defined cross section and ability to probe behavior both in the long-wavelength limit and on the scale of interatomic separations. Figure 13 shows a recent application of epithermal neutron scattering to determining the magnetic excitations in pure La_2CuO_4 , the parent of the high transition temperature superconductors. The data, which can only be obtained by inelastic neutron scattering, reveal quite conventional spin waves, but with an unusually high zone boundary energy, 0.32 eV.

Much useful and interesting work remains to be done using existing sources, although their age and condition makes it improbable that many will continue to operate into the next century. The prospects now exist, using cur-

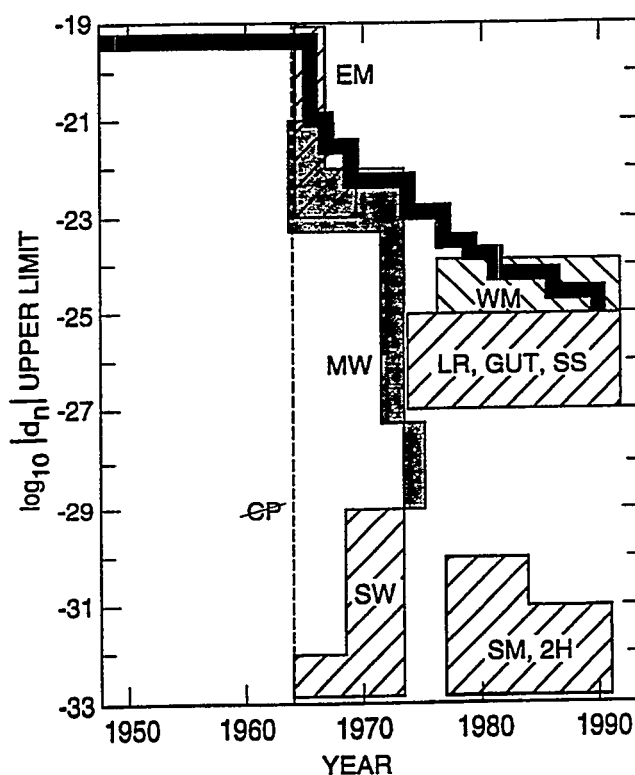


Figure 12. Upper limit on neutron electric dipole moment (EDM) $|d_n|$ versus time. Cross-hatched boxes denote the range of values for d_n predicted by the following theories: EM—electromagnetic, MW—milliweak, SW—superweak, WM—Weinberg multiple Higgs, LR—left-right symmetric, GUT—grand unified models incorporating observed baryon asymmetry, SS—supersymmetric, SM—standard, and 2H—standard model with two Higgs doublets. Figure provided by J. M. Pendlebury and G. Greene (National Institute of Standards & Technology, U.S.).

rent technology, to build new sources which will be between one and two order of magnitudes brighter than any current source. Such an increase in brightness will have substantial immediate impact in both technology and science. It will provide many new opportunities, among which follow:

1. Higher resolution spectroscopy and diffractometry revealing new effects and making possible the investigation of systems with the complexity of commercial products.
2. Parametric investigations, e.g., of temperature, pressure, and composition dependence, in areas such as ceramic and semiconductor processing.

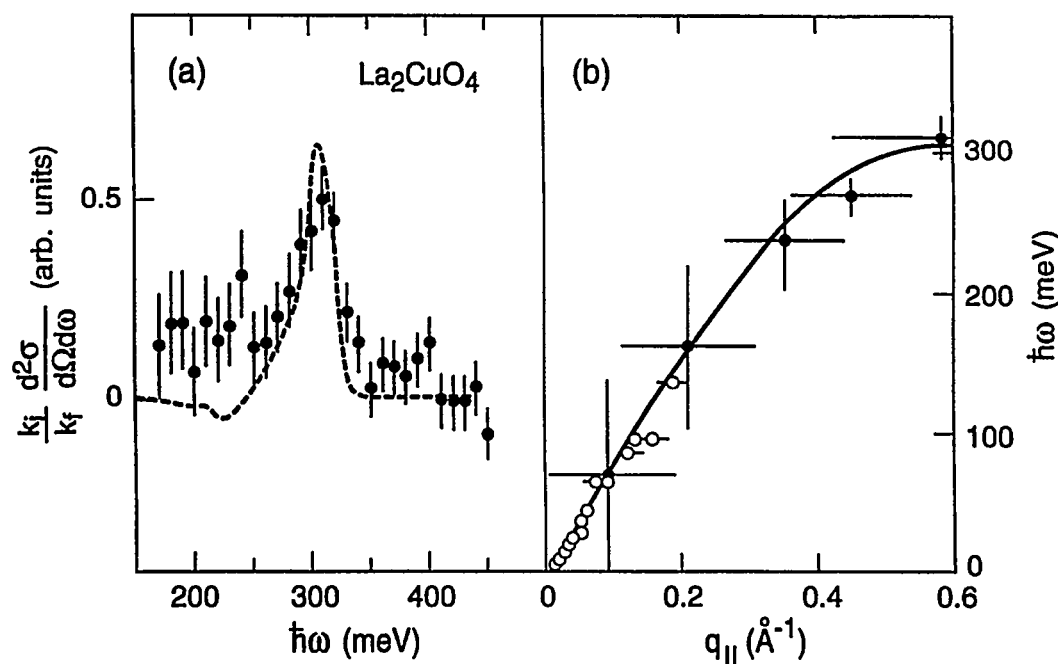


Figure 13. Zone boundary spin wave dispersion relation for antiferromagnetic La_2CuO_4 , parent of the high transition temperature superconductors. Spin waves are the magnetic analogs of collective atomic vibrations (phonons) in solids. Data were taken using the HET (High Energy Transfer) instrument of ISIS (filled circles) in the UK, and the IN1 hot source and IN8 thermal spectrometers at the ILL (open circles) in Grenoble, France. Figure provided by S. M. Hayden (Bristol, UK).

3. The possibility to examine small or dilute samples, ranging from crack tips to in-vivo systems of biochemical and medical interest.
4. The full exploitation of polarized neutrons.

Finally, past experience suggests that entirely new phenomena and uses for neutrons will emerge. Increased source strength will stimulate developments in instrumentation and techniques which will further expand the frontiers of neutron scattering, guaranteeing that this subject will have a future as productive as its past.

Acknowledgments

The author expresses his thanks to the many people with whom he corresponded on this article, most notably F. Bates (University of Minnesota), R. J. Birgeneau (MIT), D. J. Bishop (AT&T), C. Broholm (Hopkins), B. Brown (ANL), W. David (RAL), T. Holden (AECL), G. Greene (NIST), J. Kjems (Risø),

H. Mook (ORNL), R. Pynn (LANL), A. Taylor (RAL), and S. Werner (Missouri).

References

There have been several recent workshops on the future of neutron scattering. The associated proceedings provide overviews of this topic:

1. *Technology and Science at a High-Power Spallation Source*, Argonne National Laboratory report (February 1994).
2. *Report of a Review Held at Oak Brook, Illinois for BESAC Panel on Neutron Sources* (September 1992), U.S. DOE report ER-0607P (January 1994).
3. *Instrumentation and Techniques for European Spallation Source, Report of Expert Meeting Held at Cosener's House, Abingdon* (February 1992), Rutherford Appleton Laboratory report 92-040 (June 1992).

Nuclear Reaction Modeling, Verification Experiments, and Applications

F. S. Dietrich, Lawrence Livermore National Laboratory

Abstract

This presentation summarized the recent accomplishments and future promise of the neutron nuclear physics program at the Manuel Lujan Jr. Neutron Scattering Center (MLNSC) and the Weapons Neutron Research (WNR) facility. The unique capabilities of the spallation sources enable a broad range of experiments in weapons-related physics, basic science, nuclear technology, industrial applications, and medical physics.

Uniqueness of LANSCE

The Los Alamos Neutron Science Center (LANSCE) provides neutrons for the world's only facility with an active nuclear physics and technology program in the range from thermal energies to 800 MeV. In addition to the capabilities at high energy, the Proton Storage Ring (PSR) furnishes very intense fluxes of neutrons up to 100 keV that can be used for measuring cross sections on small and radioactive targets, as well as advanced applications such as dynamic radiography using neutron resonances.

For the past several years, the neutron nuclear physics program has carried out a wide-ranging program in weapons physics, basic nuclear physics, and nuclear technology. The program has had strong participation from academic laboratories and has also been enriched by "technology transfer" from the Clinton P. Anderson Meson Physics Facility (LAMPF) basic science program. An example of the latter is the use of detectors for fast neutron radiography that were originally developed for pion physics. The importance of this facility for the new LANSCE program and the breadth of potential applications are illustrated by the following examples.

Reaction Modeling and Verification Experiments for Weapons Design

In the absence of testing, improved data on nuclear cross sections are needed to ensure the reliability of weapons design activities. Many cross sections used in design have not been measured or are poorly modeled. Improving the database requires either measurements that address this issue directly or nuclear model calculations that have been verified experimentally. LANSCE is ideally suited for precise measurement of a large number of the required nuclear properties. Both Livermore and Los Alamos have initiated sensitivity studies to determine the critical needs for new measurements. Fission physics and reactions that produce or destroy tritium have been identified as areas that may have significant payoff. This program has potentially enormous impact on the ability to simulate weapons performance accurately.

Advanced Radiography

Several new radiographic techniques are currently being developed or are under study as future possibilities. In transmission radiography using high-energy neutrons, it is possible to measure small defects in light elements on the millimeter scale in assemblies. These defects are invisible in conventional photon radiography. In the successful proof-of-principle experiment at WNR, voids of a few millimeters were seen in a disc of lithium hydride sandwiched between two uranium slabs. Further experiments are planned to optimize the detector and to investigate the feasibility of computerized tomography.

First, experiments are planned this summer to demonstrate dynamic neutron resonance radiography, which uses the short, high-intensity pulses of epithermal neutrons uniquely available from the PSR. In this technique, neutrons are passed through an exploding material seeded with elements having narrow reso-

nances in the 1 to 100-eV range. The observed shift and broadening of these resonances yields information on the velocities and temperatures in the exploding material. If successful, this technique will allow characterization of the temperatures in high-explosive detonations that is available in no other way. A future additional possibility is dynamic proton energy-loss radiography, in which observation of the energy loss of high-energy protons passing through an imploding system enables the time-dependent measurement of the density profile, which is density times radius.

Accelerator Production of Tritium and Other Transmutation Technologies

For the past several years, LANSCE has been the principal experiment facility for developing the accelerator production of tritium (APT) and other transmutation technologies. Experiments have been performed to address the physics of the spallation process and the development and benchmarking of codes such as LAHET. These experiments have included measuring needed cross sections such as spallation yields and burn-up cross sections, taking measurements to test predictions of activation product yields, and testing the overall neutron performance of the codes. The facility is also important in developing and engineering practical target designs. Examples relevant to APT are the experiments to demonstrate tritium recovery that are currently under way, the planned tests of a full-scale target, and the development of beam monitoring and neutron-production diagnostics.

Radiation Oncology with Neutrons and Protons

Neutrons up to 70 MeV and protons up to 250 MeV are increasingly used in radiation therapy. At Livermore, a Monte Carlo program (PEREGRINE) is being developed to optimize dose calculations for these as well as the more commonly used photon and electron treatments. By using information from patient CT scans and a realistic description of the material composition of the human body, this technique has potentially great superiority over the current method of treatment planning based on dose measurements in a water phan-

tom. However, PEREGRINE relies on nuclear modeling calculations for neutron and proton cross sections at the higher energies, and these have significant uncertainties.

LANSCE is ideally suited for measuring critical nuclear data to verify the calculations. In fact, measurements at WNR on ^{12}C have already proven invaluable in modeling neutron reactions up to 70 MeV. A joint Livermore-Los Alamos proposal is being prepared for a comprehensive set of measurements on elements present in tissue and beam-line components using neutrons up to 250 MeV. These measurements will be directly relevant to neutron therapy and will (at the higher energies) test the techniques used to predict proton data. These data will also be important in testing the spallation-physics codes used for the accelerator transmutation applications.

Neutron-Induced Upset of Aircraft Electronics

Neutrons are the major cause of upsets and latchups in integrated circuits at aircraft altitudes. The spectrum of the WNR neutron source is excellently matched to that of the atmospheric neutron flux, but is more intense by a factor of 10^5 . The Boeing Corporation has made measurements at WNR on the components to be used in their new 777 aircraft and concluded that they have an acceptably low latchup rate. These measurements have led to an increasing usage of the facility to study the behavior of electronics components in neutron fluxes. These activities now involve six corporations.

Flux Pinning in High-Temperature Superconductors

The persistent current in high-temperature superconductors can be significantly increased by radiation damage. The damage sites pin down vortices that are needed for large-volume coherence. Fission fragments are particularly effective because of their random orientation. In a collaboration with the IBM Corporation, high-energy protons were used to fission the bismuth in samples of Bi2212 superconductor. The persistent current was increased by several orders of magnitude for a

dosage of 10^{14} fission fragments per cubic centimeter. This program is continuing with the study of other superconductors containing elements that are fissionable by high-energy protons.

The Little Boy Dosimetry Problem

Understanding the effects of neutron radiation exposure relies heavily on studies of the Hiroshima-Nagasaki bombings. There are important and long-standing discrepancies between yield calculations and dose measurements at the Hiroshima site. This problem could possibly be due to miscalculation of the neutron transport through the steel case of the Hiroshima device. At WNR, measurements have been made of transmission and scattering of neutrons using actual parts from a spare Little Boy assembly. The data are being analyzed and will be compared with calculations using the WNR spectrum as input.

Precision Measurement of Neutron Total Cross Sections

An Ohio University-Los Alamos collaboration has measured neutron total cross sections with 1% accuracy from a few MeV to 800 MeV on a wide variety of targets from beryllium to bismuth. These data, which could have been obtained nowhere else in the world, provide a severe challenge to theorists attempting to understand neutron-nucleus reactions on the basis of the fundamental interaction between two nucleons. This basic science project has an important applied spinoff by providing a database for badly needed improvement of the physics models for neutron interactions in transport codes (such as LAHET) that are used in the design of APT and other applications of spallation physics.

Acknowledgment

The work required for the preparation of this review was supported by the Lawrence Livermore National Laboratory under U.S. Department of Energy contract W-7405-ENG-48.

BREAKOUT SESSIONS

*Workshop on Defense, Basic, and Industrial Research
at the Los Alamos Neutron Science Center*

Materials Science and Engineering

Summary by T. M. Holden, AECL Chalk River Laboratories

Introduction

The science-based stockpile stewardship program emphasizes a better understanding of how complex components function through advanced computer calculations. Many of the problem areas are in the behavior of materials making up the equipment. The Los Alamos Neutron Science Center (LANSCE) can contribute to solving these problems by providing diagnostic tools to examine parts noninvasively and by providing the experimental tools to understand material behavior in terms of both the atomic structure and the microstructure. Advanced computer codes need experimental information on material behavior in response to stress, temperature, and pressure as input, and they need benchmarking experiments to test the model predictions for the finished part.

This report on the materials science and engineering breakout session summarizes the overlap between the problem areas and the expertise and tools available for their solution with neutron science at LANSCE. Several unique capabilities exist at LANSCE that we found nowhere else within the Department of Energy (DOE) laboratories. We spelled out the science and technology advances possible for materials research with a long-pulse spallation source (LPSS), and finally we considered some areas in which improvements could be made to meet customer requirements. Abstracts of some of the talks presented at the materials science session are found in Appendix C.

Overlap between Defense Programs and Scientific Capabilities

Five areas of overlap between defense programs and scientific capabilities were identified during the breakout session, which included energetic materials research, radiographic requirements, manufacturing and process modeling, polymeric materials, and radiation damage effects.

Energetic Materials Research

P. Howe described the modifications to the microstructure necessary to generate unexpected localized areas of high strain in explosive compacts. In the neighborhood of cavities or voids, high transient stresses are generated under dynamic loading just as the stress intensity factor for the static case describes stress enhancement. These stresses cause plastic deformation that generates heat locally, which can lead to unexpected detonation. Small-angle neutron scattering (SANS) is the technique of choice for characterizing the void distribution in high explosives in order to lead to a better understanding of explosive sensitivity. A program of work is already envisaged. Another area of interest is the noninvasive interrogation of the "aging" explosives by neutron diffraction to measure chemical phases present in these materials and to check for chemical decomposition and degradation of samples. D. E. Mitchell raised the issue that neutron diffraction could just as easily measure degradation and corrosion of the containment vessel.

A related problem in lightning arrester connections on which the presence of voids in the granular varistor material can lead to unwanted high electric fields was dealt with by A. Hurd. Fluctuations in density from random packing can be addressed by SANS as well as neutron diffraction (by means of intensity fluctuations in the diffracted peaks if the scale of the packing problem is appropriate, that is in the of order mms). Neutron diffraction can be used to assay cold work in the powders due to compression as well as characterizing the strains in the compacts. Work is already being done in this field. Extension of the SANS measurements to lower wave vectors, perhaps by using a Bonse-Hart spectrometer, would be valuable.

D. E. Mitchell explored why neutron radiography is a useful tool for examining packing anomalies in powder compacts. Cold neutron radiography permits greater penetration

through containment vessels if the wavelength is longer than the Bragg edge. High-energy (MeV) radiography, which is unique to the Los Alamos facilities, also permits penetration of the containing vessel. Because the shapes of the vessels are complex, tomography, that is the digital reconstruction of three-dimensional images from measurements made in transmission over an angular interval of 360° , will be important. This tomography would be a generic tool of interest to many industries.

Another exciting area in which LANSCE can provide absolutely unique data for the basic understanding of explosive propagation is the measurement of temperature by the Doppler broadening of neutron resonances with data from a single pulse of neutrons. The concept, as described by W. Trela and P. Howe, is to generate a temperature excursion by compressing the explosive at a time triggered by the LANSCE pulse and to measure the temperature at a known time after the compression by the Doppler broadening of a gold resonance from gold impurities in the materials. This experiment can be done noninvasively through the walls of a containing vessel. There is an added requirement to measure the strain in the material. The elastic strain component might be observed through shifts of the Bragg edges determined in transmission in a single pulse. Plastic strain does not have an obvious footprint amenable to determination in a single pulse.

Manufacture and Process Modeling

K. W. Mahin described the economics to be derived from accurate computer simulation of manufacturing and assembly of components, as embodied in the Smart Process technologies. Benchmarking the predictions of these simulations with experiments is clearly important. One property that has to be predicted accurately is residual stress. For example, machining a part that is subject to a stress field will cause unexpected dimensional changes as the stresses re-equilibrate. M. Bourke described the capabilities at LANSCE for measuring residual stresses at depth in engineering components noninvasively. The method has broad application not only in benchmarking for forging, welding, and casting, but also in providing basic data on materials in response to

thermomechanical processing. L. Newkirk suggested several applications of the strain techniques to welding problems and to novel fabrication schemes for U alloy components. Interest exists in extending the techniques to measure sampling volumes of order 1 mm^3 .

The alignment of the polycrystalline grains in a component strongly affects the mechanical properties. Bulk measurements of crystallographic texture are readily carried out by neutron diffractions as described by R. Wenk. It will be very important for LANSCE to routinely provide measurements from texture and orientation distribution function analysis.

C. Majkrzak described the application of neutron reflectometry to basic studies of corrosion for the case of H ingress through Ti and its oxides. This method gives very detailed information with a spatial resolution of 5 \AA and will find many applications in the area of degradation aging.

Radiography Requirement

Neutron radiography provides one effective tool for interrogating parts noninvasively to ensure their integrity. Two unique technologies are available at Los Alamos: high-energy (MeV) neutron radiography with very high penetration and resonance radiography with neutrons in the eV regime. The advantage of resonance radiography is that specific isotopes may be identified by imaging with neutrons of a particular energy.

T. Rieker raised the possibility of inspection for gases within containment vessels by means of HERA, the gamma-ray multiplicity spectrometer, via (n,γ) absorption in the gas. The possibility of gettering gases such as H and D&T within containment vessels and then interrogating the getter noninvasively by neutron scattering was suggested.

Polymeric Materials

R. Hjelm described how SANS provides a tool for probing polymeric materials via the difference in scattering of H and D. Reflectometry also provides a unique tool for examining the surfaces of polymeric materials and layered films. Studies of neutron scattering under shear

stress give important information on the strength of polymer composites. The network structure of carbon black, which vastly improves the wear properties of tires, was studied by R. Hjelm and M. Gerspacher. The project showed how a basic understanding of structure in a complex industrial material can lead to a more economic tire design.

Radiation Damage and Deterioration

Using the high flux of high-energy neutrons in the Clinton P. Anderson Meson Physics Facility (LAMPF) beam dump and the additional possibility of using the 800-MeV proton beam allow Los Alamos to accumulate test data on damage rapidly. These facilities were described by W. Sommer. Computer simulation studies of radiation damage were presented by R. Devanathan. The combination of theoretical and experimental expertise makes this a unique approach. The important aspect is to provide hot-lab equipment to examine and characterize samples after irradiation. Effort should also be devoted to preparing shielding flasks for measuring radioactive samples with spectrometers at LANSCE.

Unique Capabilities of LANSCE within the DOE Laboratories

The following unique capabilities were identified in a session after the breakout session:

- High-energy radiography for noninvasive examination of components. The facilities are unique because of the high flux of neutrons as well as their spectral distribution.
- Los Alamos expertise on plutonium metal.
- The practical possibility of temperature measurement by the Doppler broadening of neutron resonance absorption for resonances in the eV region. The usefulness is enhanced by the capability of obtaining this information from a single neutron pulse.
- The existence of high-energy and high-flux sources of neutrons and protons for radiation damage studies.
- The highest resolution time-of-flight diffractometer in North America.

The Long-Pulse Spallation Source

The possibilities for new science with a long-pulse spallation source (LPSS) were identified in the breakout session.

The fluxes from an LPSS approach those from a medium-flux reactor of order 10^{14} n cm⁻² sec⁻¹, but with a pulse length of 1 ms and a repetition rate of 60 Hz. The emphasis would be on generating a high flux of low-energy neutrons from cold moderators.

Estimates indicate that a SANS spectrometer would have 25 times more flux than the present SANS at LANSCE. This ability would permit studies of the kinetics of reactions, for example, in structural batteries. Likewise, reflectometry would benefit from a 25-fold intensity increase that would be needed to extend the wave vector range of measurements. This increase would yield higher spatial resolution. In addition, it would be easier to distinguish between models of the structure that are presently indistinguishable because of the limited wave vector range of the measurements.

High-resolution Laue diffraction from single crystals of biological molecules would open a new field for molecular structure studies at Los Alamos.

The high flux of slow neutrons could be used effectively for cold neutron radiography, for example, visualizing the oil flow within an operating engine.

Goals for Improvement

The following improvement goals were identified to meet customer requirements:

- Make texture measurement and analysis a routine service tool.
- Reduce the sampling volume in residual stress measurements to around 1 mm³.
- Reduce the wave vector range to $Q \sim 10^{-4}$ on the SANS spectrometer to make it much more useful for studying large imperfections. It was suggested that the Bonse-Hart spectrometer at Oak Ridge National

Laboratory, which is currently unused, might be set up at LANSCE.

- Improve detectors by increasing the number of detectors, borrowing new detector concepts from the high-energy physics community, and working on ways to decrease the dead time. Detector development gave more bang for the buck than, for example, source development.
- Give strong support to the benefits and developments of single-pulse science.
- Buy services within DOE for specialized applications that cannot be met at LANSCE. We recognized that it was not

possible nor cost effective to duplicate equipment at all the DOE laboratories.

Conclusion

Many areas overlap between the technical requirements for careful stockpile stewardship and the facilities available at LANSCE in the field of materials science and engineering. Many diagnostic tools for nondestructive interrogation of complex parts exist or could easily be put in place. Material characterization of structures at the atomic and microscopic scales, particularly by neutron diffraction, SANS, and reflectometry, will lead to a better understanding of the materials problems encountered in this program.

Participants

Tom Holden, Chair, AECL Chalk River Laboratories
Simon Billinge, Michigan State University
Mark Bourke, Los Alamos National Laboratory
Ram Devanathan, Los Alamos National Laboratory
Michel Gerspacher, Sid Richardson Carbon Company
Joyce Goldstone, Los Alamos National Laboratory
Mark Hedemann, Sandia National Laboratories
Rex Hjelm, Los Alamos National Laboratory
Philip Howe, Los Alamos National Laboratory
Alan Hurd, Sandia National Laboratories
James Jorgensen, Argonne National Laboratory
Kim Mahin, Sandia National Laboratories
Charles Majkrzak, National Institute of Standards and Technology
Dennis Mitchell, Sandia National Laboratories
Lawrence Newkirk, Lawrence Livermore National Laboratory
Charles O'Farrell, Sid Richardson Carbon Company
Tom Picraux, Sandia National Laboratories
Charles Prewitt, Carnegie Institution of Washington
David Price, Argonne National Laboratory
Partha Rangaswamy, Los Alamos National Laboratory
Tom Rieker, Sandia National Laboratories
James Rhyne, University of Missouri
Marie-Louise Saboungi, Argonne National Laboratory
Angus Lawson, Los Alamos National Laboratory
Greg Smith, Los Alamos National Laboratory
Walt Sommer, Los Alamos National Laboratory
Mike Stevens, Los Alamos National Laboratory
Walter Trela, Los Alamos National Laboratory
Donald Weidner, SUNY Stony Brook
Rudi Wenk, University of California, Berkeley

Soft Condensed Matter: Polymers, Complex Fluids, and Biomaterials

Summary by D. Schaefer, Sandia National Laboratories

Introduction

Historians often characterize epochs through their dominant materials, clay, bronze, iron, and steel. From this perspective, the modern era is certainly the age of plastics. The progression from hard to soft materials suggests that the emerging era will be the age of “soft condensed matter.”

The demand for easily manufactured materials with unusual combinations of properties drives a discipline encompassing polymer, complex fluids, and biomaterials, collectively referred to as soft condensed matter. Soft condensed matter often mimics biosystems—complex, multiphase, self-assemblies in which various property requirements are delegated to specific substructures.

The block copolymer was the first synthetic material based on this new concept. These hybrids are designed at the molecular level to self-assemble during processing into mesostructures. By combining hard and soft phases at the molecular level, seemingly antipodal properties such as flexibility and hardness are simultaneously optimized. Research on block copolymers is now progressing to the point that even rheological properties are controlled by synthesis. Thus, process as well as product fall to molecular engineering.

Materials derived from soft condensed matter are not necessarily soft or wimpy. Indeed, carbon-based materials hold the record for most specific properties. Body armor, for example, is made from hydrocarbon polymers.

The mythos and methods of this emerging science are not limited to solids. The design of modern lubricants, for example, exploits all the tools of soft condensed-matter science. New solid lubricants rely on the interfacial activity of tailored molecules to simultaneously achieve adherence and lubricity. Additives that

display temperature-dependent aggregation are used to control viscosity.

Neutron scattering, particularly n -angle neutron scattering (SANS) and reflectivity, is the key tool used to elucidate the relationship between structure and properties in complex systems typical in soft matter. Hierarchical structures are hopelessly overlapped in real and reciprocal space. Deuterium tagging, however, allows highlighting of specific components leading to resolution of structural details over several decades in length-scale.

Weapons Applications

Soft materials are abundant in nuclear weapons. Examples include cable jacketing, o-rings, structural elements, encapsulants, high explosives, electrodes, dielectrics, coatings, mounting pads, getters, sealants, mechanical components, printed wiring boards, gas filters, and optics. Several new surety technologies also depend on properties available using the molecular engineering tools of soft condensed matter.

Encapsulants are a good example of materials that must meet multiple requirements. Specifications for weight, modulus, dielectric constant, dielectric strength, fracture toughness, thermal expansion, and processing must all be met simultaneously. These multiple requirements are satisfied using highly filled polymer composites, processed and cured by empirical protocols.

We now face challenges regarding carcinogens that have disqualified many existing encapsulants. Attempts to eliminate carcinogens have presented a formidable challenge to weapons engineers. In the absence of a predictive model for structure-property relationships, proposed drop-in replacements with matching glass-transition temperature, elastic modulus at room temperature, coefficient of thermal expansion, and fracture toughness have failed

functional tests. Unfortunately, the science base required to understand these materials, let alone to systematically develop drop-in alternatives, is lacking. With the evolution of weapons technology into the next century, the risk associated with such ignorance will increase.

Agile Manufacturing

Polymers are the *sine qua non* of the consumer economy. In fact, the injection molding device underlies more consumer products than any other machine of the industrial age. If the weapons complex is to mimic the adaptable manufacturing processes in the commercial sector, soft materials are critical. A truly agile weapons manufacturing system is limited as much by adaptable materials as by adaptable machinery.

Many futurists believe that the tools of the cold war will not match the threats of the 21st century. In a fast-changing, information-intensive battlefield, adaptability overwhelms capacity. High-yield weapons, optimized for longevity, security, and performance, can be neutralized by unforeseen political as well as technical developments. A just-in-time weapons development and delivery system, therefore, will be more valuable than an aging stockpile.

Concepts exist, albeit nascent, to manufacture most of the nonnuclear components from soft materials. From bomb cases to signal processing devices, nontraditional manufacturing methods are conceivable. In many cases, the private sector is developing the required technologies. A 21st century, just-in-time nuclear weapon, however, requires a new materials and processing strategy.

Major Facilities

Neutron scattering is critical to realize the promise of soft condensed matter as the foundation of adaptive manufacturing. The genius of strategic planning is to recognize these critical investments and make them in a timely manner. It is incumbent on the Department of Energy (DOE), more than any other institution, to lead the planning process.

The irony of the agile production system is that its development depends on investment in the most sophisticated tools of the industrial age. Synchrotron and neutron facilities are especially important. In fact, the development of these characterization facilities was foundational to the growth of research in soft condensed matter. The precipitous decline of neutron facilities and expertise, however, threatens this most forward-focused element of the DOE research capability.

Two areas in which a long-pulse spallation source will be particularly effective are: SANS and surface neutron scattering. Both are currently (apart from neutron powder diffraction) the most widely used methods to nondestructively characterize materials at the mesoscopic level. These methods are favored in industrial research using neutrons.

SANS, for example, can be used to characterize the internal pore structure of microporous materials on length-scales from 10 to ~500 Å (or larger, if special techniques such as high-resolution Bonse-Hart systems are used). An example of an industrial application is the area of microporous membranes used for separations of fluids, where SANS has been used to characterize the internal pore morphology and spacing.

Surface neutron scattering (such as neutron reflectivity and off-specular surface scattering) is becoming an increasingly popular probe to study the structure and morphology of surfaces and interfaces, for example, of polymeric coatings, adhesives, and lubricants on solid surfaces, and of polymers and surfactants at liquid/air interfaces or at oil/water interfaces (as in research into enhanced oil recovery). Neutron reflectivity can probe the density profile of an adsorbed layer, a thin film, or a single surface to a precision of a few angstroms. Off-specular scattering can probe lateral structure, for example, roughness, islands, or pits on the surface, structural phase transitions at the interface, and so forth. Surface neutron scattering is the two-dimensional (2-D) analog of bulk small-angle scattering; however, the important difference is that only the *lateral* component of the wave vector transfer is relevant rather than the total magnitude of the wave vector transfer making it fairly easy

to resolve 2-D lateral structures up to length scales as large as 10 to 20 microns!

Role Of Neutron Scattering In Soft-Condensed-Matter Research

Composites

Advanced polymer composites have the potential to provide substantial increases in strength-to-weight. Traditional fiber reinforced composites suffer difficulties due to interlaminar debonding and stress concentration at fiber ends. A potential solution to this problem is the molecular or nanocomposite, a molecular dispersion of a rigid-rod molecule in a matrix. These polymer nanocomposites are predicted to exhibit significant increases in strength compared with conventional composites. Increases in properties have been measured as the dispersion is approached, but difficulties in processing and thermal stability have limited their performance.

New approaches to polymer nanocomposites rely on the use of liquid crystalline polymers. Experiments have relied on SANS to provide the relevant length scales and contrast needed to understand the details of the structure in these composites. The results show the formation of an interpenetrating network structure with a characteristic length scale of 8 nm. In addition, using unique contrast variation methods available only with neutron scattering, it has been found that there is substantial intermixing between the phases.

Further development of these nanocomposites will depend on the use of neutron scattering to study the details of the structure of these systems. The ultimate goal is to provide a firm basis for the design of such systems, leading to a new class of high-performance, light-weight structural materials.

In complex solids and fluids, interfaces are more important compared with bulk phases, accounting for the explosion of research based on scattering and reflection from interfaces. Indeed, self-assembled systems are often interface-dominated.

The specific adsorption of macromolecules at interfaces can provide for the tailoring of the

macroscopic response of the interface. For example, the physisorption or chemisorption of synthetically designed macromolecular species onto the surfaces can be used to modulate the physical properties (mechanical, transport, electronic, optical, and so forth) or chemical properties (reactivity, binding specificity, and so forth) of the solid/liquid or solid/vapor interface. On the other hand, the interface can be tailored to provide a template for the designed fabrication 2-D (monolayer) and 3-D (multilayer) assemblies. For example, bifunctional organic chain molecules chemisorbed at the solid/liquid or solid/vapor interface can be synthetically designed to adsorb a biological protein molecule with high specificity to thereby control the vectorial orientation and the 2-D ordering of the protein molecules at the interface.

Both synchrotron x-ray scattering and neutron scattering can be used to investigate the intramolecular structure and supramolecular ordering of macromolecules adsorbed at interfaces. For momentum transfer parallel to the plane of the interface, synchrotron x-ray scattering is probably the more appropriate technique for investigating this structure as projected onto the plane of the interface. For momentum transfer perpendicular to the interface, both x-ray and neutron scattering probe this structure as projected onto the normal to the plane of the interface. The unambiguous interpretation of such projections is facilitated by selective deuteration of particular macromolecular components or specific submolecular portions thereof in the neutron scattering case.

The proposed upgrade of the LANSCE facility to the "long-pulse" regime would provide for neutron flux densities that would greatly facilitate collecting neutron reflectivity and kinematical diffraction data for momentum transfer perpendicular to the interface, especially for enhancing sensitivity to the deuteration of specific sites in the macromolecular species. In addition, this upgrade would be especially important for enabling grazing incidence neutron diffraction for momentum transfer parallel to the interface.

Corrosion

An important potential application could be the nondestructive study of corrosion pitting at buried interfaces, for example, at metal/oxide interfaces inside electrolytes where pits can invade the metal from the oxide layer and grow from a few angstroms in size to several microns in diameter. Neutron reflectivity experiments have been done on corrosion on Ti/oxide/electrolyte systems, but so far no off-specular measurements have been done. The diffuse scattering curves represent quantities closely related to the Fourier transform of the pair-correlation function of the pit distribution across the surface and show the existence of pits under the oxide layer with an average size of 5 μ and an average separation of 10 μ . Neutrons have the additional advantage of being able to penetrate bulk solids to look at deeply buried solid/solid or solid/liquid interfaces in this manner, *in situ* and in real time.

Biotechnology

Tirrell et al. observe that "...with increasing frequency new materials or processing strategies are emerging, inspired by biological examples or developed directly from biological systems. Already, researchers are engineering bacteria or other organisms to synthesize monomers for polymer production. They are synthesizing and expressing artificial genes to produce protein-like materials with the me-

chanical properties of silk, collagen, or other materials containing elastic fibers. They are beginning to use phospholipids as templates for electronic materials; make synthetic phospholipid vesicles that, like proteins, respond to signals; use stereoselective catalyses to produce optically active polymers from racemic starting materials; and develop protein- and lipid-based sensors."¹

Often unrecognized is that a biological organism is a collection of very sophisticated soft condensed-matter subsystems. Mimicking the synthetic processes underlying these subsystems is a primary strategy of biomaterials research.

Biosystems offer important synergy between national needs. It should be remembered that the first commercial application of the transistor, now central to nuclear weapons, was in the hearing aid. Not only can biomimetic materials impact new materials for weapons, but the opposite is also true. Scientists addressing new manufacturing techniques can turn their expertise to designing better materials for biosystems such as bone prostheses.

Reference

1. Tirrell et al., *Chem. and Eng. News*, Dec. 19, 1994.

Participants

Dale Schaefer, Chair, Sandia National Laboratories
Kent Blasie, University of Pennsylvania
Elliot Douglas, Los Alamos National Laboratory
Alex Gancarz, Los Alamos National Laboratory
Paul Gilna, Los Alamos National Laboratory
Rex Hjelm, Los Alamos National Laboratory
Alan Hurd, Sandia National Laboratories
Charles Majkrzak, National Institute of Standards and Technology
S. K. Sinha, Exxon Research & Engineering
Greg Smith, Los Alamos National Laboratory
Sandra Zink, Los Alamos National Laboratory

Fundamental Neutron Physics at LANSCE

Summary by G. Greene, National Institute of Standards and Technology

Introduction

Modern neutron sources and science share a common origin in mid-20th-century scientific investigations concerned with the study of the fundamental interactions between elementary particles. Since the time of that common origin, neutron science and the study of elementary particles have evolved into quite disparate disciplines. The neutron became recognized as a powerful tool for studying condensed matter with modern neutron sources being primarily used (and justified) as tools for neutron scattering and materials science research. The study of elementary particles has, of course, led to the development of rather different tools and is now dominated by activities performed at extremely high energies. Notwithstanding this trend, the study of fundamental interactions using neutrons has continued and remains a vigorous activity at many contemporary neutron sources. This research, like neutron scattering research, has benefited enormously by the development of modern high-flux neutron facilities. Future sources, particularly high-power spallation sources, offer exciting possibilities for continuing this research.

The scientific content of this research, which has come to be known as "fundamental" neutron physics, has important implications for particle physics, nuclear physics, astrophysics, for testing fundamental phenomenology, for determining fundamental constants, and for investigating the underlying symmetries of nature. In addition to their scientific importance, activities in this field have led to a variety of technical developments that have found extensive utility in other neutron activities. Neutron guides, modern neutron polarizers, as well as a variety of neutron detectors that originally developed as a consequence of fundamental neutron activities are now widely employed at all modern neutron sources. Continuing instrumentation developments, which have a significant impact on materials science studies, include novel methods of neutron po-

larization (based on optical pumping of ^3He) as well as intense sources of extremely low-energy neutrons (ultra-cold neutrons [UCNs]).

In anticipating a program of fundamental neutron physics at the Los Alamos Neutron Science Center (LANSCE) and Weapons Neutron Research (WNR) facilities and future sources, it is useful to note that the character of such research is qualitatively different from typical neutron scattering activities and materials science studies. While most neutron scattering measurements use installed, fixed instruments (perhaps with some modification), fundamental neutron physics experiments often employ rather complex apparatus specifically constructed for *one measurement*. Often, such an apparatus will require several person-years for development and construction. It will often require capital investments on a scale not very different than that required for a scattering instrument even though it will be used for data acquisition for a period of months. With rare exceptions, the support for constructing and operating apparatus is provided by outside funding and is not directly provided by the neutron facility itself.

An experiment in this field often arises from the realization that an interesting problem, perhaps in a field such as astrophysics or particle physics, is best addressed, or is only addressable, at an intense neutron source. This insight is likely to develop among researchers outside the traditional neutron physics community. It is not uncommon for projects in this field to be "technique" driven in that they develop through the realization that a method from some other field can be applied to neutrons with good effect. There have, for example, been very fruitful interactions with the atomic physics, optics, and low-temperature physics communities.

An intense neutron source should be viewed as an important resource for the broad scientific community. This contact with a very broad scientific community has important positive

implications for the tenor of scientific and technical activities that may be expected at LANSCE and WNR. The fundamental neutron physics community is diverse and includes many researchers with the highest international scientific reputations. A vigorous program in fundamental neutron physics at LANSCE and WNR and future sources at Los Alamos will encourage important scientific connections with an extremely broad scientific community.

As an aid in the review of this research area, it is convenient to divide fundamental neutron research into three categories:

- *Fundamental and particle physics with cold neutron beams* concerns elementary particle physics, tests of fundamental symmetries, and the determination of fundamental constants using neutron beams.
- *Particle physics with stored UNC's* concerns research with neutrons of sufficiently low energy that they can be "trapped," held, and studied in material bottles for long periods (minutes).
- *Epithermal and higher energy neutron physics* research concerns activities using neutrons having energies ranging from about 1 eV to energies of tens or hundreds of MeV.

This classification is by no means rigorously distinct. Many activities span more than one category. Such overlap is an important feature of this area of research; the field of fundamental neutron physics is actually a rather broad interdisciplinary endeavor. A high degree of "cross-fertilization" between different areas of physics has been essential to the vitality of this research.

Fundamental and Particle Physics with Cold Neutron Beams

Fundamental research with cold neutron beams includes a rather considerable variety, and it is beyond the scope of this summary to provide a complete review. Aside from focusing on a few specific and somewhat arbitrary highlights, this section will present only a brief survey of the field. More detail is readily available in the

form of the proceedings of a series of international workshops and conferences¹⁻⁴ that have been devoted to this work.

In general, there are two reasons why cold neutron beams are well suited to studying the neutron and its fundamental interactions. Experiments that measure static neutron properties (including decay properties) or the interaction of free neutrons with laboratory fields typically benefit from the (relatively) long observation times (of flight) that are available with low-energy neutrons. Experiments that require spin-polarized neutrons profit from the relative ease with which intense cold beams can be polarized with high efficiency.

Accurate values for the properties of the free neutron, determined using cold neutron beams, have implications in many fields. The determination of the neutron magnetic moment can shed light on the quark structure of the nucleus. Limits on the neutrality of the neutron reflect on the more general question of the neutrality of matter and indirectly on the gauge invariance of the electromagnetic interaction. Measurements of the correlations in free neutron decay can shed light on the origin of parity and time reversal symmetry violation as well as providing important information on the nature of semileptonic weak interactions. Measurements of the neutron beta decay lifetime are useful for detailed tests of the standard model of the weak interaction and provide a parameter of great importance in astrophysics and cosmology. The measurement of selected neutron cross sections is important for stellar astrophysics and understanding the details of the standard solar model. Measurements involving polarized neutrons have shed light on the details of the weak interaction between quarks. During the last decade, the search for a baryon nonconserving "oscillation" (in parameter space) between the free neutron and its antiparticle, the antineutron, has been interesting.

Particle Physics with Stored Ultra-Cold Neutrons

Measurements of the neutron electric dipole moment d_n , and the beta decay lifetime of the neutron τ_n , which are possible using neutrons

of extremely low energy (UCNs⁵⁻⁷), have proved to be extremely valuable in achieving a better understanding of the symmetry breaking components of fundamental forces. The neutron is now viewed as a composite structure comprising two "down" quarks and one "up" quark bound together by the strong interaction. In spite of the neutron's electric charge neutrality, the electromagnetic force (10^{-2} times the strength of the strong force) manifests itself with a nonzero neutron magnetic moment. Neutron structure is also influenced by the "weak" interaction that, although its strength is 10^{-7} times that of the strong force, leads to neutron beta decay. The weak force has a "handed" character that leads to the violation of parity symmetry P (as far as we know, this is not the case for the strong and electromagnetic forces). Neutron decay, like most beta-decays, is a parity-violating phenomena. The relative "weakness" of the weak force is responsible for the relatively long neutron lifetime of approximately 888 ± 2 s.

In 1964, experiments on the decay of the K^0 mesons revealed another even weaker force that violates both parity and time reversal symmetry T. This force, which is perhaps 10^{-12} times the strength of the strong force, would also be expected to play a role in the internal structure of the neutron. In view of this minute strength, other manifestations of this force have so far proved, not surprisingly, to be elusive. Thus, it has been difficult to develop a theory for the force or to even determine whether it is a new interaction or simply a novel manifestation of other interactions. The simplicity of the neutron makes it an attractive tool for the study of T violation.

The P and T breaking symmetry properties allow the possibility of permanent electric dipole moments (EDMs) in elementary particles. Naively we may anticipate that the size of the neutron EDM may be $d_n \leq 10^{-12}$ times the diameter of the neutron. That is, $d_n \leq 3 \times 10^{-26}$ e cm (note that the present, most widely favored explanation for the T violation predicts much smaller effects, with d_n being 5 to 7 orders of magnitude less). From experiments with stored UCNs, the present 1σ error is 4×10^{-26} e cm. There is a strong incentive to improve this precision.

The weak force with a relative strength of 10^{-7} is more accessible and consequently it is much better understood. It exists by virtue of exchange of the known heavy W^+ , W^- , and Z^0 particles, and it is related in detail to the electromagnetic force in the "electroweak" theory. Beta decay is its most direct manifestation at low energies, and the decay of the neutron is the simplest case for which quantitative low-energy measurements can be made. The neutron lifetime τ_n and the asymmetry parameter for the correlation between the decay electron momentum vector and the neutron spin direction furnish simultaneous, linearly independent inputs that can be solved for the parameters g_V and g_A , which represent the strengths of the vector and the axial vector parts of the weak force for the nucleon. The same value of g_V , with some small corrections, will apply to all nuclear beta decays and to the decay of the muon. The shortage of precision in the neutron measurements has frustrated the pursuit of the finer details of this theory. In the last 5 years, measurements with stored UCNs have improved the precision of τ_n by nearly an order of magnitude and the consistency between different experiments has been improved. In the future, the asymmetry parameter may also be measured using UCNs. Further improvements by a factor of 10 are highly desirable for both quantities as they will then provide one of the most stringent tests of the standard model for the weak interaction.

Compared with thermal and cold neutron speeds of approximately 2000 m/s and 500 m/s, respectively, UCNs have speeds less than about 6 m/s. They can be stored in "bottles" with material walls (or confined by laboratory magnetic fields). During storage, they steadily disappear from the bottle because of beta decay and loss processes involving nuclei in the wall surface. Average storage times of hundreds of seconds can be obtained with clean, room-temperature walls of suitable materials. During storage, the neutrons continually bounce between the walls of the storage vessel, reflecting elastically from the walls, and may cross the bottle many thousands of times before being lost. Observation times for individual neutrons in UCN experiments may be hundreds or even thousands of seconds. These times may be contrasted with observation

times that are restricted to tens of milliseconds for cold beam experiments. This huge advantage is partly offset by lower counting rates, but the net improvement in precision can still be several orders of magnitude. In addition, UCN storage vessels can be displaced by several meters from the source line of sight, which results in very low background conditions. Nonetheless, the low absolute count rates associated with all UCN measurements have resulted in nearly all experiments being limited by counting statistics. All UCN measurements will therefore profit from the higher UCN densities that are possible at advanced neutron sources. Indeed, the most exciting prospects for fundamental neutron physics at the next-generation neutron source likely will involve the use of UCNs.

At present, the most intense source of UCNs in the world is at the Institut Laue-Langevin. The number density of UCNs up to the speed of 6 m/s at the output of the turbine blades is about 90 cm^{-3} . Another intense source is at the WWR-M reactor of the Petersburg Nuclear Physics Institute (Russia) where the density is about five times less, reflecting the comparably lower source thermal neutron flux. These sources have been in use since 1986, and these institutions have no immediate plans for more intense sources.

A spallation source with the characteristics of LANSCE could provide UCNs that might be competitive with the best sources in the world. This source would be based on the down conversion of thermal neutrons by back reflection from a moving crystal. The source involves a rotor using Bragg reflection from crystals of an synthetic fluorinated mica (or perhaps graphite). Such a device downconverts neutrons with a wavelength of approximately 10 \AA from the cold source at the *peak* intensity in the pulse. This source is in the detailed design stage and is hoped to be installed for tests at LANSCE in the near future.

Down-scattering in superfluid helium or solid D_2 is an extremely exciting alternative method of UCN production, which could offer densities approaching 10^4 UCN cm^{-3} if employed at the 1-MW long-pulse neutron source under consideration in area A. This technology offers the possibility of a two order of

magnitude increase in UCN density, which would truly revolutionize the field of UCN research. Such a source, if shown to be practical, could lead to very significant advances in fundamental neutron research and could open a variety of opportunities for studying materials with UCNs.

Epithermal and Higher Energy Neutron Physics

Epithermal neutrons and neutrons at higher energies from pulsed-accelerator spallation sources can be employed to provide sensitive tests of parity and time reversal invariance. The energy resolution obtained using time-of-flight techniques offers the possibility of observing and using p-wave resonant enhancements of parity nonconserving effects. A particularly novel use of energetic neutrons examines the average enhancement in several p-wave resonances in a compound nucleus. From such averages, taken over many nuclei, it is possible to extract weak meson-nucleon couplings. This information provides a unique window on the nature of the weak interaction between nucleons.

The information from this class of observations can be enhanced by better understanding the details of the resonances that lead to the large observed enhancements. Such information could be obtained using a gamma ray detector array. The installation of such an array at LANSCE would provide a powerful new tool for investigating the weak interaction as well as a variety of other phenomena.

The broad spectrum of neutrons available at WNR offers the possibility to carry out measurements at much higher neutron energies. At WNR, it is possible to obtain data as a function of incoming neutron energy in a single experiment for neutrons between 100 keV and 600 MeV. This energy regime bridges the gap between low-energy reactions, where compound nuclear processes dominate, and high-energy reactions, where any compound nucleus formation is preceded by extensive intranuclear cascade-type particle emission. Consequently, many studies can be conducted at WNR to provide important information on reaction evolution.

Neutron-proton bremsstrahlung is important both as a fundamental measurement needed to understand photon emission in medium-energy heavy-ion reactions and as a mechanism for studying meson-exchange contributions to the nucleon-nucleon potential. This is important complementary information to that obtained by the deuteron photodisintegration measurements at the Continuous Electron Beam Accelerator Facility.

Charge-exchange (p,n) and (n,p) reactions can be studied using protons and spallation neutrons, respectively. Direct (n,p) reactions induce Gamow-Teller similar to those of β -decay but over a much wider range of excitation energies. Substantial differences are observed between the data and calculations that include correlation effects.

Much nuclear data for numerous applications can be obtained at spallation sources: cross sections of charged particle emission (dosimetry and neutron therapy), fission and (n,xn) cross sections (shielding, transmutation facility design), photon yields, detector calibration, explosives and drug detection, oil-well logging, and so forth. These issues are discussed at length in the reports of other groups.

Summary

The development of intense neutron sources has seen the parallel development of a rich research program in which the neutron (and its fundamental interactions) are the object of study. This research, employing a rather wide variety of experimental approaches and techniques, has produced results of importance in particle physics, nuclear physics, determining fundamental constants, astrophysics, and studying fundamental quantum phenomenology. While the scope and sensitivity of this research has expanded with the refinement of

measurement techniques, it is a particular characteristic of this area of study that advances in both the quality and quantity of results follow directly from improvements in source intensity.

LANSCE and WNR provide unique facilities for investigating many issues. The proposed long-pulse facility, which would employ the full linac beam, could provide an unparalleled source of UCNs and project Los Alamos into a position of world leadership in the area of fundamental neutron physics.

References

1. *Fundamental Physics with Reactor Neutrons and Neutrinos*, T. von Egidy, Ed. (Institute of Physics, 1977).
2. *Proceedings of the Workshop on Reactor-Based Fundamental Physics*, B. Desplanques, F. Gonnwein, and W. Mampe, Eds. (*J. Physique Colloque C3*, 1984).
3. *The Investigation of Fundamental Interactions with Cold Neutrons*, G. L. Greene, Ed. (National Bureau of Standards Special Publication 711, U.S. Government Printing Office, 1986).
4. *Proceedings of the International Workshop on Fundamental Physics with Cold Neutrons*, D. Dubbers, W. Mampe, and K. Schreckenbach, Eds. (*Nucl. Instr. and Meth. A284*, 1989).
5. L. Koester and A. Steyerl, *Neutron Physics* (Springer-Verlag, 1977).
6. V.K. Ignatovich, *The Physics of Ultra-Cold Neutrons* (Clarendon Press, 1990).
7. R. Golub, D. J. Richardson, and S. Lamoreaux, *Ultra-Cold Neutrons* (Adam Hilger, 1991).

Participants

Geoffrey Greene, Chair, National Institute of Standards and Technology
Tom Bowles, Los Alamos National Laboratory
David Bowman, Los Alamos National Laboratory
Avigdor Gavron, Los Alamos National Laboratory

Andre Michaudon, Los Alamos National Laboratory
Chris Morris, Los Alamos National Laboratory
Ron Nelson, Los Alamos National Laboratory
Sue Seestrom, Los Alamos National Laboratory
Lee Schroeder, Lawrence Berkeley Laboratory
Terry Taddeucci, Los Alamos National Laboratory
John Ullman, Los Alamos National Laboratory
Steve Wender, Los Alamos National Laboratory

Applied Nuclear Physics in Support of SBSS

Summary by D. Strottman, Los Alamos National Laboratory

Introduction

Since the advent of the 800-MeV proton linear accelerator over 3 decades ago, the facilities on the Clinton P. Anderson Meson Physics Facility (LAMPF) mesa have pioneered many developments that provide unique capabilities within the Department of Energy (DOE) complex and in the world. New technologies based on the use of the world's most intense, medium-energy linac, LAMPF, are being developed. They include destruction of long-lived components of nuclear waste, plutonium burning, energy production, production of tritium, and experiments for the science-based stockpile stewardship (SBSS) program. The design, assessment, and safety analysis of potential facilities involve the understanding of complex combinations of nuclear processes, which in turn establish new requirements on nuclear data that transcend the traditional needs of the fission and fusion reactor communities. Other areas of technology such as neutron and proton therapy applications are also placing new requirements on nuclear data. The proposed Los Alamos Neutron Science Center (LANSCE) now under discussion combined with the appropriate instrumentation will have unique features and capabilities of which there were previously only aspirations.

Gamma-ray spectroscopy is fundamental to experimental neutron science. The white source of LANSCE, coupled with a large-scale gamma-ray detector array, is a unique powerful combination for neutron science. This combination is the preferred tool to meet many nuclear data requirements, including the Advanced Fission Model, (n,xn) cross sections on ^{239}Pu and other elements mentioned in this session, plus data requirements we have not yet anticipated. Finally, this combination impacts all neutron science and ensures a leadership role for LANSCE.

In this paper, I will first discuss some of the physics issues—with emphasis on the applied arena—that can be investigated with the

LANSCE upgrade and then discuss some of the many applications that can be addressed with this unique facility. Abstracts from speakers at this breakout session are included in Appendix D.

Physics Issues

It is no surprise that an accurate knowledge of fission cross sections is important to the SBSS program. Our knowledge of neutron-induced fission cross sections, the fission daughter products, gamma, and fission branching ratios, and so forth is meager and not widely appreciated. Additional knowledge of these items is needed for the actinide and transactinide nuclei, e.g., the fission cross sections of the heavy uranium isotopes.

Considerable work is also required for the subactinide nuclei. Work aimed at extending one's knowledge of the fission process to nuclei lighter than uranium has made initial progress, but there is no systematic characterization of the subactinide nuclei. As an example, the fission physics and characterization of fission fragments of Pb and W is badly needed for the accelerator production of tritium (APT) and accelerator-driven transmutation technologies (ADTT) projects. In this and other projects, measurements in conjunction with a gamma detector array will greatly improve knowledge of the physics.

As is not uncommon, the boundary between purely applied science and basic research is blurred. In neutron physics, this is particularly so. Knowledge gained from a study of the nucleus often has direct application, and vice versa. Two examples of this follow.

In the first example, neutron-rich nuclei are produced as fragments following fission. Use of the (n,f) reaction (including targets of exotic or isomeric nuclei) will provide an extremely rich source of new nuclides. Combined with HERA, the gamma-ray multiplicity spectrometer, this will allow spectroscopic studies

of fission fragments as a function of E_n . Almost no fission-fragment gamma-ray spectroscopy experiments have been performed (except for a few at Daresbury) so this is largely unexplored territory. It will also allow spectroscopic study of other nuclei in regions previously unstudied. Use of γ - γ or $\gamma\gamma\gamma$ correlations will lead to an unprecedented ability to extract previously inaccessible information. As such, the LANSCE and HERA facility will complement heavy ion-induced reactions and the proposed radioactive beam facilities.

A second example involves studies of states with large deformation in the second and third well using (n,γ) or (n,f,γ) . Study of superdeformed states with heavy-ion reactions is an exciting frontier in nuclear physics. Superdeformed states in the actinides are typical and have been known for some time as fission isomers or states in the second or third well. However, the physics of these states is incompletely or poorly understood. States in the second well typically have a 2:1 deformation ($\beta = 0.6$) and those in the third well have a deformation of 3:1 or $\beta = 0.8$. Many of the nuclear structure problems that exist for the superdeformed states with $A < 200$ also exist here, but the fission isomers are complementary in that they have low spin. Earlier work has raised several puzzles, e.g., the microscopic calculations of the fission barrier have not been uniformly successful suggesting our knowledge of the nucleon-nucleon interaction needs revision. Further, it is known that intermediate structure resonances in the second well cannot be described within the conventional picture; this suggests our understanding of the nuclear potential energy surface is inadequate.

There is a whole range of neutron-induced reaction physics that needs to be addressed at LANSCE and the Weapons Nuclear Research (WNR) facility. Neutron scattering observables such as measurements—including spin observables—for optical model development and reaction cross sections for APT are required. Study and validation of preequilibrium reactions/models are badly needed and would be possible from the data acquired; these models are essential to obtain data for the transport calculations for APT design, neutron radiogra-

phy, and radiation oncology. More information is needed for dosimetry and radiation standards. A study of multiparticle final states including all produced particles following neutron scattering is needed for the APT and ADTT projects. Benchmarking measurements for validating computer codes are essential. Integral measurements of t/p , n/p , ... are required as well as measurements of spallation product distributions including radioactive yields for APT. Additionally, a better characterization of the nuclear properties of unstable nuclei subsequent to neutron scattering or neutron-induced fission is needed for both basic physics as well as for APT, ADTT, and the weapons program. Measurement of (n,xn) reactions, e.g., $^{239}\text{Pu}(n,xn)$ and $^{239}\text{Pu}(n,xn,\gamma)$, is needed for the weapons database.

Increasingly, there is a need for comprehensive neutronics and radiation analyses of nuclear systems that involve particle energies greater than 20 MeV, currently the energy limit for neutron reactions in the U.S. national nuclear data system, ENDF/B. There will be a strong synergism between weapons' issues and medium-energy applications, e.g., APT and neutron radiography. Measurements will lead to theoretical model development and improved predictive capabilities of the applied programs.

Specific Applications

Physics for Defense Programs

Several speakers mentioned experiments that would improve our predictive capability of a nuclear weapon's performance and how to better understand problems associated with an aging stockpile. Among these is the data effort to better understand past Nevada Test Site events. This effort must include both better characterizing prompt diagnostics and a better understanding of rad-chem diagnostics. Many of the required cross sections for rad-chem detectors used in the past are poorly known or suspected of being inaccurate. The use of LANSCE for transmutation of wastes was discussed by J. Zumbro. Finally, there was a discussion of measurements relevant to proliferation concerns on actinides, transactinides, and structural materials. Many of these issues were also discussed in detail at the classified session.

During the breakout session, D. Madland presented his new Advanced Fission Model for use in applications. Post-scission (i.e., after the snapping of the neck between the two nascent fission fragments) observables currently used in applications include average total fission-fragment kinetic energy E_{tot} , average prompt fission neutron multiplicity, (E_n) , average prompt fission neutron spectrum $N(E)$, and the average fission fragment (A, Z) and its corresponding neutron cross sections. All of these post-scission fission observables are distributions. However, in almost all applications, only average values for these distributions are used. The essence of the Advanced Fission Model is to replace average values of post-scission observables by the distributions of these observables together with their correlations. The Advanced Fission Model will require using experimental measurements combined with extensive modeling of the fission process. Detailed measurements will be required of

- the cross section for fission as a function of incident neutron energy
- detailed mapping of the fission products, including
 - a) the isotopic identification of the fragments
 - b) energy spectrum of emitted neutrons $N(E)dE_n$
 - c) kinetic energy of fragments $E_x(f)$

Radiography, Both Static and Dynamic

The promise of neutron radiography was discussed by several speakers. High-energy neutrons have considerable penetrating power and are more sensitive to low-Z materials than are other techniques. A. Gavron and C. Morris spoke on using highly penetrating high-energy neutrons to probe for small defects or gaps in materials. Based on a detector having a flat response and seeking a signal 5 s above background in a reasonable time period (hours), the optimal neutron energy range for radiography is 8 to 400 MeV. Gavron discussed a proof-of-principle experiment. In it one detected pinholes of 4, 8, and 12 mm diameter in a 2.5-cm sheet of LiD sandwiched between two 5-cm-wide blocks of ^{238}U . There was excellent comparison between a Monte Carlo simulation and the observation.

Gavron also discussed advanced concepts possible with a dedicated facility, and what would be required of such a facility. With the appropriate setup, one could perform neutron tomography by rotating the sample about an axis and taking multiple exposures. A second possibility is to exploit the energy dependence of neutron scattering to search for defects in materials. Morris also discussed possible new, position-sensitive detectors for neutrons.

J. Lynn spoke on the potential of using resonant radiography at LANSCE. The resonant cross section of a neutron interacting with a material is dependent on the temperature of the sample: the higher the temperature, the broader the resonance. Thus, a pulse of neutrons passing through a sample generated, e.g., by an explosion or a dynamic shock, can measure the temperature of the sample. Resonant radiography can be used to find minute impurities in a sample by searching for the resonance of the impurity. It was also mentioned that different areas of a sample could be seeded with different trace elements and thereby provide spatial and temporal information of a shock.

Medical Applications

Radiation has long been an effective tool in the fight against malignant tumors. Several radiation oncologists have been exploring the usefulness of protons and neutrons in this struggle. Despite much work the effective radiation dose on a tumor in a human is inaccurately known. Further, the optimal energy—which will depend on the nature and location of the tumor—of the incident radiation is not known. There are too many interfaces and density changes (e.g., organ boundaries, bones, etc.) that may cause an incident particle to scatter, or induce secondary radiation. It was originally proposed by a group at Los Alamos, and as discussed by M. Chadwick, now being carried out at Lawrence Livermore National Laboratory (LLNL), to model the transport of the incident and secondary particles using modern transport codes such as MCNP or Peregrine in a human. Treatment regimens may be individualized and determined by modeling using CAT scan images. Besides reliable transport models, one needs very accurate data up to 250 MeV or higher for both neutron-

and proton-induced reactions on a variety of target nuclei including carbon, oxygen, calcium, and nitrogen.

Chadwick and P. Young discussed the importance of developing neutron and proton cross section libraries in the incident particle energy range of 20 MeV to approximately 200 MeV for transport applications. They described new theoretical methods for developing cross section libraries at these higher neutron and proton energies including a new model for calculating multiple preequilibrium effects. Currently, an intranuclear cascade plus evaporation model is used in the LAHET code to calculate nuclear data for all neutron interactions occurring at energies greater than 20 MeV. Use of the intranuclear cascade model at energies below 150 MeV is known to be inappropriate, and this procedure is followed primarily because of the unavailability of reliable cross section data at energies above 20 MeV. Chadwick and Young described a collaborative effort involving personnel from LLNL and Los Alamos to improve the nuclear physics information, particle transport capability, and overall reliability of the nuclear analysis code systems. They described how such measurements can be combined with theoretical calculations to obtain (n,xn) cross section information needed for defense and other applications that is otherwise sparse or unavailable.

Industrial

Several industrial applications of neutrons were discussed. J. Ullman discussed using neutron-induced fission for pinning down the vortices that are needed for large volume coherence in a high-temperature superconductor. As a result one can obtain much higher, persistent currents at high magnetic fields.

S. Wender presented applications of LANSCE for single-event upsets (SEU) and multiple-event upsets, an important concern in avionics as more electronics with decreasing feature size are incorporated into guidance and control systems. One specific example involved certifying the chips used in the Boeing 777 fly-by-wire system. The WNR 30° spectrum resembles that caused by cosmic rays at altitudes of 30,000 to 50,000 ft, but with an intensity of 10^5 greater. Thus, by exposing the chips to

the WNR neutron beam, one can in a very short time determine the susceptibility of the chip to SEU over the expected service of the plane.

As an example of the applicability of LANSCE to the study of radiation damage to materials, G. Logan described a putative experiment to understand dose-rate effects at the National Ignition Facility (NIF). Ideally, one would design structural materials that are impervious to radiation or do not become highly radioactive in an inertial confined fusion of Tokamak reactor. For this one needs to know the nonlinear effects of high doses, i.e., multi-transmutation steps, nonlinear effects on annealing rates of piled-up voids, and for NIF, the effect of short-pulse gamma bursts on the transmissivity of laser optics. With a combination of irradiation of samples at WNR and modeling (to account for the different neutron energy spectrum between WNR and NIF), it is hoped that considerable knowledge of material response may be gained.

Instrumentation

To fully use the new capabilities, it is imperative to obtain the necessary instrumentation. New position-sensitive detectors are being designed to permit high-resolution radiography.

The combination of LANSCE and a large-scale detector array for gamma-ray, x-ray, and neutron detection would be a very powerful combination and facilitates many measurements. For example, one could measure all the quantities needed in the Advanced Fission Model excluding the fragment kinetic energies; these latter can, however, be estimated if the detector array also has the capability of neutron measurement. A multidetector array with large resolving power for gamma-ray detection is the key component because mapping the Z,A and excitation of each fission fragment requires coincidence of gamma-ray measurements of the correlated fragment pairs.

A new array could be built at a cost of 10- to 15-million dollars over 2 years. An alternate route would be to bring a large-scale gamma-ray array, e.g., HERA, to LANSCE. HERA is one of three large-scale arrays in the U.S. and

is available because the more advanced GAMMASPHERE has been built at the Lawrence Berkeley National Laboratory (LBNL) 88-Inch Cyclotron. A proposal has been made to LBNL and DOE/OHENP to site HERA at LANSCE.

Never before would such a powerful detector have been combined with a neutron source. It will uniquely enable one to address problems of interest to SBSS. Other detectors required to execute the program are a large-angle particle array and a neutron detection array.

Conclusion

In this breakout session, many new and exciting applications of an upgraded LANSCE were presented. Some of these possibilities—such as radiography, fission studies, dosimetry measurements, code benchmarking—are already in the exploratory phase. Other possibilities such as using neutrons to determine temperature or density profiles of shocked materials or to measure fission branching ratios await further accelerator or detector development. The known and many unconceived uses of neutrons promise an exciting future in many applications.

Participants

Dan Strottman, Chair, Los Alamos National Laboratory
John Becker, Lawrence Livermore National Laboratory
Tom Bowles, Los Alamos National Laboratory
Mark Chadwick, Lawrence Livermore National Laboratory
Frank Dietrich, Lawrence Livermore National Laboratory
Avigdor Gavron, Los Alamos National Laboratory
Damon Giovanielli, Sumner Associates
Paul Lisowski, Los Alamos National Laboratory
Grant Logan, Lawrence Livermore National Laboratory
John Lynn, Los Alamos National Laboratory
Dave Madland, Los Alamos National Laboratory
Andre Michaudon, Los Alamos National Laboratory
Chris Morris, Los Alamos National Laboratory
Ron Nelson, Los Alamos National Laboratory
Sue Seestrom, Los Alamos National Laboratory
Stephen Sterbenz, Los Alamos National Laboratory
John Trabert, EG&G
John Ullman, Los Alamos National Laboratory
Steve Wender, Los Alamos National Laboratory
Phil Young, Los Alamos National Laboratory
John Zumbro, Los Alamos National Laboratory

Condensed Matter Physics and Chemistry

Summary by W. J. Nellis, Lawrence Livermore National Laboratory

Introduction

The proposed Los Alamos Neutron Science Center (LANSCE) upgrade is ideally suited for science-based stockpile stewardship (SBSS) because LANSCE is a high-intensity pulsed neutron source located at a nuclear weapons design laboratory. The attributes of a high-intensity pulsed source are essential for performing experiments on Pu and other materials important for SBSS. Neutrons can accurately probe thick bulk specimens, probe thin layers both freestanding and embedded in thicker specimens, and provide time-resolution for some phenomena. Both ordered structures and disorder in solids, liquids, and amorphous materials can be characterized, as well as phase transitions. Because LANSCE is at a nuclear design laboratory, specimens important for SBSS issues are available. Los Alamos National Laboratory is an appropriate place to develop the requisite hardware to accommodate SBSS specimens, such as Pu.

In some cases, new and more detection systems need to be developed to obtain the necessary accuracy within the available neutron counting times. It is also important that an appropriate technician staff be available to assist in operating the instruments. The capital and operating costs of neutron detection instruments are small compared with the cost of neutron sources and efficient detection systems necessary to achieve the potential of LANSCE.

The proposed facility is primarily for SBSS issues, but it would also be rich in related industrial and scientific applications.

Upgrading LANSCE is strongly recommended because the neutron scattering and SBSS communities need to

- have a neutron-scattering facility dedicated to the wide range of experiments
- emphasize high intensities to probe small samples, such as Pu

- emphasize high resolution in neutron instrumentation
- use high-intensity short neutron pulses to time-resolve phenomena such as phase transitions in Pu

Other recommendations for LANSCE include

- coupling the neutron pulses and spectrometers with other apparatus that produce extreme conditions, such as a high-pressure cell and pulsed high-magnetic fields
- maximizing detector number and efficiency before increasing beam intensity because detectors are much less expensive than increases in beam intensity
- operating the facility efficiently to attract industrial users

The details are summarized in the written input of the speakers in Appendix E.

Specific Issues of SBSS Importance

Plutonium and the Actinides

Equation-of-state (EOS) and vibrational-spectra data of Pu, its alloys, and the light actinides (Pu, Np, U, and Th) are needed to improve the accuracy of the EOS of these materials for calculations related to the weapons stockpile. Experimental data are needed at static pressures up to 100 kbar and temperatures up to 1500 K and higher, if possible. The Pu²⁴² isotope should be used to minimize neutron absorption and sample heating. Relatively small samples are necessary because of the relatively small sample volumes in high-pressure cells, safety issues in handling Pu, and Pu²⁴² is a rare isotope. High intensities are needed for small samples. The α -, β -, and δ -phase solids and the liquid should be studied. Phonon spectra are needed in the solids, and structure factors are needed in the liquid, which are obtained by inelastic and elastic neutron scattering, respectively.

Solid Pu has the most complex phase diagram of all the elements. It was determined by x-ray scattering over 30 years ago. Explaining it would be a tremendous scientific accomplishment. Six solid phases at room pressure are reduced to only two phases by 2.5 GPa (25 kbar). The melting temperature is reduced from about 900 K to 780 K by 2.5 GPa. Phonon spectra are needed to calculate thermal pressure and to look for lattice instabilities in the solid that might explain this incredibly complex phase diagram. Powder diffraction experiments are needed to verify the known phases, identify any possible unknown phases, and determine Debye-Waller factors, compressibilities, and thermal expansions. Methods to determine disorder within ordered systems should be developed to shed light on mechanisms driving phase transitions. Time resolution available with a pulsed source might be able to determine the time required for one solid phase to transform to another. A detection system more efficient than the present one is needed for the diffraction experiments.

Measurements of phonon spectra require single crystals of α -, β -, and δ -phase Pu. The β and δ phases need to be stabilized by something like ~1% of Np and Ga, respectively. Several small crystals with the same orientation might be grouped to effectively form one large crystal. Single crystals of Pu are difficult to grow but the scientific information to be obtained justifies the effort. Phonon spectra have not been obtained for any material at high pressure, which means the technique needs to be developed with relatively simple simulants, such as Al, Cu, and Ta.

Studying the systematics of the light actinides (Th, U, Np, and Pu) is recommended to bring enhanced understanding to all of them.

Liquid Pu is anomalous in the sense that near ambient pressure Pu contracts on melting, at 2.5 GPa Pu has no volume change on melting, and at higher pressures Pu expands on melting. Accurate interatomic potentials should be derived from neutron-measured liquid structure factors to determine the scientific causes of this anomalous behavior and to calculate thermal pressure accurately. A new detection system is needed to be able to perform these experiments in the liquid. Such a detection sys-

tem would have applications to industry and to scientific issues, such as structures and interactions in amorphous magnetic systems and the nature of glasses in industrial and geological materials.

Structural determinations of liquids require dedicated diffractometers covering a high-Q range with short-wavelength neutrons, detectors at low angle $2\theta < 45^\circ$, and a comprehensive data analysis procedure. Advanced chopper spectrometers being designed and built at spallation sources (PHAROS at LANSCE and MARI at ISIS in the UK) are extremely valuable for studying liquid dynamics. Low-angle detectors to measure a large range of energy transfer at low Q are especially important in systems undergoing phase transitions.

Clearly, the study of Pu is important. S. S. Hecker, Director of Los Alamos National Laboratory; J. Immele, Director of Nuclear Weapons Technology Programs at Los Alamos; and R. Fortner, Associate Director of Physics and Space Technology at Lawrence Livermore National Laboratory (LLNL) all emphasized the importance of Pu studies for SBSS in their presentations the first day of this workshop. Thus, it is important to consider pulsed neutron-scattering experiments on Pu at high shock pressures. However, shock experiments on Pu are not now possible. Independent of LANSCE, complementary dynamic high-pressure experiments have been proposed for the Los Alamos "Pu gun," and these need to be performed. However, the Pu gun has been available at Los Alamos for many years and has never been fired with Pu samples. No technological reason prevents Pu gas-gun experiments from being performed safely. When it is actually possible to do experiments on Pu at high shock pressures, then a careful consideration of possible pulsed neutron experiments at LANSCE on Pu at high shock pressures would be warranted.

Hydrogen

Hydrogen samples at several 100 kbar up to the Mbar range have a volume of about 10^{-6} mm^3 . While hydrogen is an important SBSS material and a strong neutron scatterer, these tiny samples in diamond anvil cells

would require very high neutron intensities, not currently envisioned.

Shock-Induced Structures and Defects

The purpose of this application is to

- take advantage of the high intensities at LANSCE to understand shock effects in complex Earth materials that surrounded underground nuclear explosions
- understand a case of "knob twisting," which is the process of making a computer code agree with experiments by tuning a parameter in a simulation code to obtain agreement with experiments without providing a physical basis for the agreement
- develop a collaboration between LANSCE and LLNL on shock-compression experiments

Underground nuclear explosions at the Nevada Test Site were done in tuff, a multiphase, SiO_2 -rich water-saturated rock. Treaty Verification issues, weapons effects in rocks, and the containment of underground nuclear explosions would be better understood and, perhaps, controlled if the structure of the rock surrounding an explosion were known as a function of shock pressure diverging from the source of an explosion. Thus, it is important to determine the glass and/or crystal structure of tuff shocked to pressures up to the 100 GPa (Mbar) range. Because about 80% of tuff is Si and O_2 in the form of silicates, pure SiO_2 quartz ideally simulates complex tuff. Tuff and quartz should be shocked with a gas gun at LLNL up to Mbar pressures and recovered for characterization of crystal structure and defects at LANSCE. LLNL has developed sophisticated techniques to recover samples intact from shock pressures up to the Mbar range.

Shock-wave temporal profiles in tuff measured at LLNL have been interpreted in different ways by two different groups. Both interpretations are obtained by matching two different computer models to the same experimental data. Physically characterizing the structure of this material on recovery from high shock pressure is the only way to resolve the discrepancy in the two computer models. Because

of the many phases in shocked tuff and quartz, high intensities at LANSCE are needed.

Similar information about shock-induced defects should be obtained for materials whose mechanical constitutive properties are needed for accurate computational simulations under shock loading driven by high explosives. Examples include shocked uranium, lead, tantalum, and steels. Characterization of shock-induced defects are needed to develop constitutive models from first-principles theory. Defect densities in shocked materials could probably be determined by low-angle neutron scattering.

Shocked quartz is the only material in which two different glasses can be made in the same material at the same time with the same chemical composition. Thus, neutron scattering in shocked quartz might provide insight into the nature of a glass, an important technological and geological material. In superconductors, shock-induced lattice defects increase intragranular critical current densities by increasing magnetic fluxpinning energies. LANSCE would be useful to determine defect densities in shocked superconductors, which could then be correlated with critical current density.

These applications would not only enhance LANSCE capabilities but would also enhance shock-wave technology. Unique structures are generated by shock deformation, and shocked materials have never been characterized by neutron scattering.

Dual-Use Techniques for SBSS and for Scientific/Industrial Users

Local Structures on Different Time Scales and Short-Range Order in Complex Materials.

There is a possibility of resolving local structures on different time scales using neutron powder diffraction. This capability is important in understanding phase transitions, the glass transition, and any property of a lattice in which the structure observed depends on how fast the sample is probed. The time scale of an experiment depends on energy resolution. Thus, it should be possible to vary time scale by varying energy resolution. Pulsed neutrons and a chopper spectrometer can be used

to vary energy resolution by measuring the dynamical structure factor $S(Q, w)$ over a wide range of scattering vector Q and energy transfer w . Suitable integration yields the total structure factor $S(Q)$ and the pair distribution function (PDF). By combining the energy resolved scattering and the PDF technique, it is possible to resolve the structure over a wide range of length and time scales.

Preliminary measurements have been made using the MARI spectrometer at ISIS. The available Q resolution is insufficient, and it is impossible to obtain adequate beam time for the required development, especially for U.S. scientists who have no priority at this European-Japanese facility. The proposed Phase II development of the PHAROS spectrometer at LANSCE will yield a machine with Q -resolution superior to that at MARI, which would access the range of (Q, w) required for these experiments. The proposed PHAROS upgrade will make LANSCE the primary facility in the world for this kind of measurement. The method could also be focused on understanding phase transitions in Pu.

In addition, a technique yet to be developed needs high-intensity neutron fluxes to obtain short- and intermediate-range structural information for complex materials. The method would solve local arrangements of atoms in disordered materials, such as glasses and liquids, or in materials with a disordered component to the structure, such as Pu approaching a phase transition or shocked quartz. The technique requires measurement of PDFs from neutron powder diffraction patterns. The development of this technique owes much to work that has been done at LANSCE. This method has already been applied successfully to perovskite structures, including high-temperature superconductors. Because structure determines physical properties, the method is a possible technique to guide the synthesis of novel materials, as well to understand the nature of existing ones. The method might also yield information about the energetics of defects, the mechanism driving martensitic shape memory alloys, and optimal structures in high-temperature superconductors. This method uses high fluxes and high resolution.

Fine-Scale Textures in Complex Electronic and Other Materials. A class of materials of current importance are soft-condensed-matter and complex-electronic materials. Properties of interest include electronic, optical, and magnetic ones. These properties are controlled by intrinsic inhomogeneities or textures on multiple and hierarchical space and time scales. These textures are in the mesoscopic domain between the microscopic and macroscopic scales; quantities of interest are magnetic domains, grain size, and so forth. Intrinsic fine-scale textures refer to precursor structures, superlattices, polaronic distortions, and so on, which are the result of intrinsically coupled, and often competing, microscopic interactions, such as spin, charge, and lattice.

Examples of the types of condensed matter whose mesoscopic structures are important to their physical properties include plutonium's aging and microstructural response to external perturbations, perovskite ferroelectrics, high-temperature superconductors, colossal magnetoresistance materials, shape-memory alloys, self-assembling polymers, and macromolecular heterostructures. Neutron scattering data from spallation neutron sources at ISIS are revolutionizing local-structure information in high-temperature superconductors. PDF analysis and energy resolved PDF analysis need to be enhanced to become major new tools to determine mesoscopic structures of the types of materials mentioned. Accelerator-based pulsed neutron sources are an essential element in understanding and controlling the structures of such materials, which in turn tunes their physical properties.

Industrial Research: Catalysts and Hydrogenous Materials. E. I. DuPont researchers have used neutron powder diffraction to refine crystal structures of new phases of aluminum fluoride to find alternatives to chlorofluorocarbon catalysts. Detailed atomic structures are needed to develop explanations for why such compounds react chemically as they do. These crystal structures were obtained using both neutron and x-ray powder data on microcrystalline powders. Neutron scattering is sensitive to low- Z elements, such as H, C, and O, and x-rays are especially sensitive to high- Z elements. Similar experiments are performed on polymers and high-temperature oxide super-

conductors for the same reason, namely, to obtain scientific understanding of materials for developing possible new products.

Future efforts are expected to focus on heterogeneous catalysts under real operating conditions, 2000 psi (13 MPa) and 350°C. To run a successful catalyst program, DuPont needs a user facility that can accommodate a large quantity of chemical apparatus and safe operating procedures to handle potential chemical hazards under real operating conditions. In addition, prompt-gamma and inelastic neutron scattering also hold promise for studies of catalysts. If DuPont is to find LANSCE useful, single-crystal structural studies will need to be more routine and will need to handle smaller crystals, and high fluxes and more efficient detectors are needed. Because of DuPont's emphasis on its core polymer business, studies of polymer systems, especially those designed to complement synchrotron x-ray studies, will benefit from neutron investigations. Dupont would like a capability to convert automatically neutron scattering powder diffraction data into PDFs. Neutron tomography is a possible new area in which to investigate manufactured products for defects.

In his presentation, R. L. Harlow of Dupont spoke about Department of Energy (DOE) user facility/industrial interactions. His talk was entitled "Let's Get Real." To this observer, his presentation was motivated by the statements made the previous day by M. R. C. Greenwood of the Office of Science and Technology Policy and a question to people from industry, namely, "who should pay for the scattering experiments they want?"

M. R. C. Greenwood said that large companies should be requesting support of the U.S. government for an enhanced neutron scattering facility at LANSCE, rather than Los Alamos National Laboratory requesting support as it is currently done. Harlow said that if Dupont were asked to speak for a neutron facility, their first question might be "what's a neutron?" Rather than playing the role of spokesperson, DuPont as a company would probably get out of neutron scattering experiments had they not signed formal agreements to perform experiments at DOE facilities for some length of time. He described a downward

spiral at Dupont, essentially aimed at increased profitability in the short term, which includes a large decline in "basic research," namely, efforts aimed at understanding materials as a basis on which to develop new products; release of chemical engineers (the company "motto" is "better living through chemistry"); retirements, layoffs, and moves to academia or national laboratories by skilled researchers; few jobs for new graduates; and the possibility that all research might be contracted out of DuPont.

Harlow's view of DOE user facilities is that DOE is hostile to industrial users and that DOE facilities are too inefficiently operated to be really useful to an industrial user. He said that the only beam lines operated efficiently are those operated by companies. He was saying that DuPont has essentially no interest in doing neutron scattering experiments, and when Harlow does do them, DOE facilities make it difficult for him.

With respect to payment, Harlow said that DuPont has already invested 2-million dollars in beam lines and has yet to receive scattering results for this money. If he asked his company for more money for occasional exploratory research, his request would be turned down. He said he needs ready and quick access to scattering facilities to perform preliminary exploratory investigations on materials to determine their viability for potential applications. Because of what DuPont and Harlow have already contributed in money and effort, he does not think he should pay for access for occasional exploratory research.

Harlow was one of a few representatives from industrial laboratories at the meeting. His remarks are similar to what I have been told by researchers from other major industrial laboratories. His statements are also consistent with the impressions that other conference expressed in the corridor after his presentation.

Hydrogenous Earth Materials. Water was essential for the origin of life on Earth, and for volcanic, tectonic, and erosional processes that have shaped the Earth's surface and interior. To understand the role of water and hydrogen in the evolution of the Earth, it is necessary to know how mineral phases retain hy-

drogen under varying environmental conditions from ambient to high pressures and temperatures. Neutron scattering is necessary to investigate hydrogenous and aqueous mineral phases and their stability at high pressures and temperatures because neutrons are sensitive to scattering by H and O atoms. The fundamental issues in earth science require the same capability to subject hydrogenous minerals to high pressures and temperatures at a high-intensity neutron source as Pu.

Pulsed Neutron Measurements of Magnetic Excitations. Magnetic spin interactions can be studied using pulsed time-of-flight spectroscopy. The method is especially suited to one-dimensional magnets in which the chain axis is aligned parallel to the direction of incident neutrons. The application of this method to KCuF_3 has provided detailed information on the dynamical correlation functions of the underlying model system and supports the theoretical picture of "spinon" excitations. These experiments were performed at the MARI chopper spectrometer at the ISIS pulsed neutron source in the UK. Similar experiments could be done at LANSCE with the appropriate spectrometer.

Unique magnetic scattering experiments could be produced at LANSCE by coupling the high magnetic fields available at Los Alamos to a pulsed high-intensity neutron source. That is, a pulsed magnetic field could be synchronized to the neutron pulse. Using magnetic fields up to 20 to 30 Tesla would alter magnetic and electronic structures, which could be probed uniquely with pulsed neutrons to characterize potentially new classes of materials.

An even more novel experiment would be to do neutron scattering off a sample both at high pressure and in a pulsed high-magnetic field. Both pressure and magnetic field change electronic and magnetic structures. Investigating the effects of both would be scientifically exciting.

Magnetism in Metallic Superlattices and Magnetic Correlations in Disordered Magnetic Systems. A significant fraction of the worldwide magnetism research community is currently involved in the study of metallic super-

lattices. Neutron scattering is uniquely suited to probe magnetic interactions because of the magnetic moment of the neutron. Magnetic superlattices comprise alternating layers of a magnetic element and a nonmagnetic spacer layer. Phenomena under study include a giant magnetoresistance, interlayer exchange coupling, and strain and magnetoelastic effects on phase transitions. The question of a phase-coherent coupling of the spins in the magnetic layers across the magnetically "dead" layers has been a particularly intriguing part of these investigations. The neutron scattering techniques of reflectometry and wide-angle elastic diffraction are important for understanding magnetic interactions in superlattice systems. Superlattice perfection, interface roughness, magnetic moment distribution, and so on are probed by neutron reflectivity. Wide-angle elastic diffraction provides information on coherence effects and incommensurate magnetic structures.

Improvements in wide-angle elastic scattering from magnetic multilayers would be useful. Multilayer film samples are essentially high-quality single crystals but with small volumes. For example, typical thicknesses range from less than 400 Å up to 5000 Å. Perhaps, improvements might be made with better instrumentation and increases in detection area.

Intense interest has been generated recently in nanostructural materials in which there are short length scales (~100 Å) of chemically and magnetically ordered structures embedded in a uniform matrix. Magnetic ordering can be studied by small-angle neutron scattering, which can lead to determining the length scale of the magnetic order and whether or not the spin ordering is static or dynamic. The instrument to study nanostructured magnetic systems requires a relatively wide Q-range and high intensity for the small particles. The wavelength dispersion and time structure of a pulsed source should enhance the scattering from magnetic nanoparticles.

Development of methods to investigate small nanostructural powders would also mean that smaller Pu samples could be studied at higher pressures. That is, increasing pressure requires decreasing sample size.

Participants

Bill Nellis*, Chair, Lawrence Livermore National Laboratory
Simon Billinge*, Michigan State University
Alan Bishop*, Los Alamos National Laboratory
Ram Devanathan, Los Alamos National Laboratory
Richard Harlow*, E. I. Dupont
Mark Hedemann, Sandia National Laboratories
James Jorgensen*, Argonne National Laboratory
Angus Lawson*, Los Alamos National Laboratory
Christian Mailhot, Lawrence Livermore National Laboratory
Charles Majkrzak, National Institute of Standards and Technology
Steven Nagler*, University of Florida
Charles Prewitt*, Carnegie Institution of Washington
James Rhyne*, University of Missouri
Jim Schirber, Sandia National Laboratories
Galen Straub, Los Alamos National Laboratory
Joe Thompson, Los Alamos National Laboratory
Walter Trela, Los Alamos National Laboratory
Robert Von Dreele*, Los Alamos National Laboratory
Don Weidner, SUNY Stony Brook

*Speaker

The Use of Neutron Scattering in Nuclear Weapons Research

*Summary by R. J. Juzaitis, Director, Applied Theoretical Physics Division,
Los Alamos National Laboratory*

Introduction

We had a weapons science breakout session last week. Although it would have been better to hold it closer in time to this workshop, I think that it was very valuable. It may have been less of a “short-sleeve” workshop environment than we would have liked, but as the first time two communities—the weapons community and the neutron scattering community—got together, it was a wonderful opportunity to transfer information during the 24 presentations that were made.

Before I came here, I checked my viewgraphs with classification, and they suggested some minor changes. A lot of the issues that need to be raised can be discussed in an unclassified format.

I heard comments from people in the neutron scattering community that they understood better what the physics issues were in terms of nuclear weapons performance and what is bothersome to the designers as they work within a challenging environment. On the other hand, people from the weapons community commented that it was interesting to see the great diagnostic techniques that are available to look at a part of the physics regime with which they are interested. Most of our experience with sophisticated diagnostics was on downhole experiments at the Nevada Test Site (NTS). The workshop was a great meeting of the minds, and I think that it is necessary for us to continue this collaboration.

I would like to thank Steve Sterbenz, who did a lot of the footwork required to get these two communities together in the same room at the same time. A lot of valuable information was exchanged.

The New Design Paradigm

Since we talked earlier about cosmology and associated philosophies, I am going to discuss the philosophy underpinning the new design paradigm that we are considering in the weapons community. What kind of challenges face us in dealing with a diminishing stockpile that is still the underpinning of our national security? Vic Reis and John Immele mentioned six pillars that will underpin our nuclear weapons program in the future; I will refer to the first three.

First—weapons performance. We anticipate the need to recertify or requalify old components in the enduring weapons systems as they age. “Weapons performance” involves the need to make very informed and good judgments about systems that are in stockpile and the need to “raise a red flag” to the policy community when we have a problem. Second—“weapons science” relates to the science-based stockpile stewardship (SBSS) aspects that are being discussed here. And third—“enduring stockpile options” addresses how we preserve the capability when there is no requirement to design and replace a device. As Vic was showing, these build requirements come and go. We have a slow period between now and early in the 21st century in which we are probably not going to build. However, if the stockpile does remain at a flat or low level, there will probably have to be some replacements in response to aging problems and safety/surety concerns. How do we preserve the capability to do this credibly? SBSS has been proposed as an enabling concept.

In the design community, we had to go one step further to find a new design paradigm that would establish the flywheel for our activities in the next few years. In this

regard, I want to focus on the importance of integral nuclear testing in the past and aboveground differential experiments in the future. In the past, the whole design paradigm was really geared toward a nuclear test. We had very good computational and local experimental infrastructures, but the way we used them was preparing for the underground test.

The nuclear test was the integrating element for the program. It got people interested in important problems and also accurately focused our activities and allowed us to design weapons for the stockpile that we could certify within certain constraints. The designs subject to these constraints were tested in Nevada. We could then say that the physics package would have a reliability factor of "one." There was no statistical basis for establishing these confidence limits. They were based on judgment and linked to an integral experiment. We did the design work and did some integral experiments at the NTS, which gave an explosive yield reflecting the combined effect of multiple, complex physics processes. We would argue that "yield plus judgment" would allow us to certify the weapon performance in the stockpile.

We are now in a new paradigm in which we do not have this integrating element. We need to control the growth of the error bars associated with assessments or how various things influence the performance of a weapon system. Those error bars will not give us the confidence that we had with nuclear testing. The goal is to mitigate the growth of the error bars. The best way is to use these differential experiments conducted at aboveground experiment facilities—the Los Alamos Neutron Science Center (LANSCE) being one, and explosive hydrotesting being another—and to link them with computing. Computing will become the new integrating element and the basis under which we will establish confidence. This puts special weight on our computer code development and on the physics models that go into them.

The FADES Project

This new paradigm does not make all of the past test experience worthless. What has become a favorite acronym in the design community is FADES. It stands for the "Fundamental Analysis of Documentation of the Enduring Stockpile." The enduring stockpile was designed in an era of nuclear testing. As we proceeded through the nuclear test program, our codes and diagnostic measurements at Nevada challenged each other. There was a dynamic interplay between what you could calculate and what you could measure at Nevada. Both of the capabilities were quite developed at the time underground tests were cut off. A lot of our calculational advancements came about near the end, but most of the devices in the stockpile were certified on the basis of much simpler experiments at Nevada and much cruder calculations.

Now, if we consider the present situation, we note that current calculations and calculational tools embody a lot more detail that was not available when the "enduring stockpile" was designed. This is particularly true of the physics models employed in the simulation codes. FADES is methodically and rigorously applying the most modern computational analyses to archived nuclear test data. The object is to predict more consistently the diagnostic record of these tests. In so doing, the complete set of diagnostic measurements recorded on a given event together act as a constraint on the physics models. Calculations are required to consistently explain the complete body of data. Associated "attributions" of specific physics models to specific diagnostic data must be carefully identified and scrutinized. In the past, empirical factors normalized to integral measurements provided computations with significantly less predictive scope because details of specific physical processes were not included. In an era of nuclear testing, when we needed to predict only to the next test or to a slight extrapolation from tested regimes, such computational tools sufficed. Today, much more predictive

capability is required. FADES will help us to identify which physics processes require more careful and precise simulation fidelity. Classification concerns restricts my discussion of the details of these physics processes.

We are going to reanalyze the archived set of underground test data. In doing so with our modern computational models, we will start identifying the "missing physics." Things that we used to treat empirically, we could get away with because we were in more interpretive and extrapolative mode than in predictive mode. We can take this "missing physics" and propose new experiments, for example, ones that can be done at LANSCE that will allow us to study a physics process in isolation. Then we will take this new data, improve the physics models, which are now the integrating link, and validate them. The models become extremely important here because not only do we have to match the aboveground experiment (AGEX) data, but we have to explain better archived underground test (UGT) data. Stewardship compels us to "look back" to make sure that our codes are not drifting away from the integral experiments that we were able to conduct in Nevada. Then all of our assessments, or the design of any prototype weapon, would be based on a fundamentally more predictive model.

LANSCE's Contribution to Weapons Physics

So what "pieces" of weapon physics can LANSCE provide? There are quite a few. As a result of the discussions on Friday and Monday, we came out with a list. This list is not meant to be exhaustive. If we had to choose the most important item that could quickly show the benefit of LANSCE experiments, what would we pick?

Materials science is absolutely important in the absence of nuclear testing because we have to be able to predict compressions of a fissile material. From those predictions, we must infer nuclear reactivity of the device with a computational "bridge."

To attribute the right aspects of the physics to the right phenomena, material science has to be understood better. We have to know how much of our inability to predict compressions is because we do not understand material strength and how much is because we are not computing explosive burn or hydrodynamics right.

Plutonium equation of state is extremely important, and there is not a great deal of data, particularly in the above-100-kilobar regime. The characterization of the phonon spectrum of plutonium using the diffractometry techniques that have been discussed here would allow us a theoretical bridge to the equation of state. The phonon spectrum tells us about the interatomic potentials and this can be related to the equation state of the material. This is a more indirect approach. You could take a piece of plutonium, go out to TA-55, shoot a gas gun, and infer the equations of state through Hugoniot measurements—which we have not done. This is a slow process, and data are not coming in a huge stream right now. LANSCE provides a complementary approach to come up with the same information that we desperately need—the plutonium equation of state.

We have talked about the strength modeling of plutonium. If you have an overdriven and really robust system with a huge high-explosive energy, the material properties lose importance, and the problem can be treated hydrodynamically. To first order, we treated everything like fluids. Unfortunately, some of the optimized designs that we have now in the stockpile do not have super robust systems in terms of driving energies. In this lower energy regime, material strength actually presents a major issue for understanding the details of implosion.

Material strength is important, and anything we can do to find out about strength, particularly using diffraction techniques, gives us good insight. In addition to plutonium, other materials make up a pit. In an implosion system, plutonium—because of its nature—may be the softest material in the combined set of shells. Near the end of

an implosion when plutonium is behaving like a fluid, the material properties of the other materials become dominant. We have to understand the other material strength properties too.

Dynamic materials behavior is important because there is a great interest not only in a static sense (crystal structure), but in a dynamic sense. How does it change? How does the crystalline texture respond to mechanical deformations? We are talking about strain rates in the range of 10^4 to 10^5 per second, which means you need a resolving power in your measurement that says things happen within a microsecond window. I have heard a lot of talks that imply this should not be a challenge. This is good, because this is what we need.

Plutonium is a very perverse material in that it has a large number of "phases." We try to stabilize it, but we do not always have control over the phases during various parts of the dynamic process of implosion. Phase transitions are also important in a static configuration. As a device is sitting in stockpile for many years, it goes through a temperature cycle. You can consider the whole stockpile-to-target sequence as a kind of temperature fluctuation. What happens to materials after they sit for 20 to 30 years through these temperature cycles? Are there locations in the material that have gone through a phase transition while others have not? In a static sense, does that put residual strains in materials that express themselves as microdefects? You would never have a chance to explore these microdefects until you actually dynamically test a weapon, which is a real challenge. The dynamic behavior of materials that results from a phase transition in the static (waiting) configuration is important.

Spallation is Critical to Understanding

Material spallation is another critical issue for weapons designers. Unanticipated spallation in the class of designs currently making up the enduring stockpile can re-

sult in a "dud," if significant enough. In the past, we went to Nevada many times without fully appreciating the effects of spall on the quality of the resulting implosion and burn, nor having a great deal of ability to ascertain to what extent spallation was occurring in early phases of the implosion. As we analyzed local hydrodynamic data—pin data—to discern the quality and symmetry of implosion, a great deal of "ragged behavior" in the time-of-flight record was attributed to spallation of the inner shell. But we never had a good predictive physics model for the development and evolution of spallation. However, if severe enough, spallation could result in a quenching effect on the thermonuclear reaction processes and possibly dud the entire weapon. This is important information for which we need a better handle.

How is spallation influenced with aging? Helium resulting from alpha decay builds up with time in the metal. How do these helium voids coalesce under dynamic conditions? Do they create a path to spallation? Are we more susceptible to spallation? The answer is probably "yes." To understand the spallation process is critical, which means that you really have to look at impurities and voids in a metal and study its aging and temperature cycle. How do these helium bubbles migrate with temperature gradients or temperature cycles? Once you subject the metal to a dynamic situation, what happens to all of the helium bubbles and how do they predispose your system to that phenomenon.

Dynamic damage evolution is important. If you have something that is predisposed to spall, can you dynamically test it and look at 10 microsecond intervals to see how the damage or the defect progresses to a point where it would be unacceptable?

Finally, there is the issue of temperature and plastic flow. If we can actually deform a material, look at its strain, and correspondingly get an idea of what temperature increase accompanies the strain, we may have another way of looking at strain rates or measuring strain rates. This is ma-

terials science. Not exhaustive, but these are critical points.

Weapons Safety Assessments

High-explosive initiation is very important from the standpoint of weapons safety assessments. Right now the state of the art in modeling weapons is to capitalize on heterogeneous reactive burn models. The heterogeneous reactive burn modeling (I will not get into the details) involves first looking at the explosive as bulk material. Particular "hot spots" relate to intergranular voids in the high-explosive material. Upon passage of a shock the mechanical deformations would facilitate the transfer of mechanical energy to thermal energy. Here you get localized high-temperature spikes, which would facilitate initiation of the explosive. We would like to model this predictively to get an idea of what these hot spot temperatures are, and to understand the sensitivity of an explosive to shocks and other insults.

Accident assessments, just by their nature, are very scenario dependent. You cannot test every particular accident scenario. You must use a computational tool just to satisfy the environment, safety, and health (ES&H) constraints. You do not want to be blowing up things all of the time. The ability to predict the sensitivity of an explosive to various insults that relate to some microstructural change in the explosive is critical to understanding the explosive response. Then you can approach the "grand challenge" calculation, the ultimate response of the whole weapons system to some specific accident scenario. Neutron resonance radiography, using a metallic dopant, is very key, and we are definitely interested in this approach to measuring hot-spot temperatures.

Another important use of LANSCE may revolve around enhanced surveillance of actual stockpile units—the detection of defects or voids in low-Z components of the weapons physics package. The penetrating power of high-energy neutrons

makes them an excellent tool for discriminating low-density defects or voids when these occur in low-Z material sandwiched between high-Z material. High-energy neutron radiography is critical to being able to survey units that have not been disassembled or cannot be disassembled due to limited numbers of stockpiled units. Nondestructive inspection is a very attractive aspect of this technique.

In the classified breakout session, F. Mortensen showed some dramatic examples of the kind of defect that can occur in low-Z materials in certain weapons components. We do not really understand them because they are three-dimensional in nature, which relates to the computational challenge. Modern weapons were designed as two-dimensional devices, but imperfections are three-dimensional and sometimes are very localized. Who knows what the result in performance degradation is? This is another "grand challenge" problem. To make sense of this, you need to know when the problem is there. In a small stockpile, the Navy is very jealous about every unit that it has. It cannot tolerate you coming and chopping up a weapon to understand the "parts." You have to be able to do this nondestructively. The high-energy neutron radiography is definitely a tool we need to pursue.

Applied Nuclear Physics Requires Cross Section Information

D. Strottman mentioned a lot of applied nuclear physics issues. I singled one out in particular because I got excited about it just last week.

In the general area of applied nuclear physics, we still need cross-section information. The database is not complete. Why do we need this information? Not because we are designing new, exotic weapon systems, but because we need to understand for the FADES process the radio-chemical data that has been accumulated through many years of underground testing. By deciphering the neutron fluxes, you learn where the energy in the weapon

actually evolved. It gives you a much better understanding of the performance of a weapon exploded in the underground test. Not all the cross sections are well understood. We need more measurements.

As I mentioned, near the end of the nuclear testing era, we started returning a lot of great time-resolved, energy-resolved diagnostics, which we did not have the time to assess carefully. We now need to go back and look at some of these in a more idealized experimental configuration to understand what happened. A lot of these diagnostics relate to neutron conversion—either converting a neutron that comes out of a device to a gamma ray or looking at proton recoil. The details of those interaction processes are not completely understood, but LANSCE experiments may provide insight. To unfold the information about the neutron at the point of origin, which is crucial, we have to understand our measurements to get the original source strength or intensity of neutrons, and where they originated.

Fission Models Need Refinement

Finally, I was very intrigued by the proposed fission model refinement. In the codes that we have now, we look at fission as an “average process.” We look at the products of fission as “average fission fragments,” an “average number” of neutrons emitted. To be predictive, we would like to replace those average values of these post-scission observables with distributions and their appropriate correlations. What are the actual fragment masses produced in the fission? How do they relate the incident neutron energy? What are the kinetic energies carried by these fission fragments in what distribution and what are the actual neutron multiplicities?

One step further, what makes this particularly exciting is the transport of fission fragments in a charged media. These fission fragments may actually have knock-on reactions with other atoms or clusters of atoms in an exploding device that can

influence the behavior of a very critical aspect of device performance.

When we discuss weapon performance from the standpoint of empiricism, we never truly understand the exact significance of specific physics factors in establishing the performance margins of boosted weapons. To what extent is hydrodynamics a factor? To what degree are impurities important in quenching reactions? Characterization of the importance of fission-fragments in the overall physics behavior of the weapon may help to resolve part of the overall puzzle.

Establishing Teams on Collaborative Projects

I think what we started this week is very important, but where do we go from here? It was a necessary and sufficient condition to get these two communities to talk to each other. We need to establish teams on collaborative projects that look at the five areas that I mentioned. We have a resonance (not a pun) between the neutron scattering capabilities to measure certain observables and the weapons design community’s need to have those things measured, understood properly, and integrated into advanced simulation code. For those issues, can we actually form collaborative projects? We need for this to happen.

Another issue is “dynamic” versus “static” experiments. Almost universally, when you ask the weapons folks what can they do with neutron scattering, they will say “static is good, but dynamic is better.”

When you talk about dynamic experiments with energetic materials (high explosives or hazardous materials), you really have to consider containment and think about ES&H and security. However, those considerations should not become a road block that prevents us from attacking the technical challenges. But they need to be confronted up-front in the process, so we do not get caught with what happened to the Dual-Axis Radiographic Hydrodynamic Test (DARHT) facility. If environmental issues are not given sufficient

consideration in today's highly charged political climate, or even if there is such a perception, political agendas will come into play to thwart all the great technical plans that were identified for a given facility.

In terms of an international user facility, there are going to be constraints and tradeoffs. We have to develop a team approach so we can do the critical experiments. For these collaborative projects and the whole suite of experiments that are proposed for LANSCE, what percent of beam availability can we count on? We

need to state the amount of availability, and ensure that critical milestones in Defense Programs research plans can be met in a timely way.

Finally, a practical consideration. A point-of-contact in all of the technical divisions, funded by nuclear weapons technology, may be useful. These points of contact would be useful to Steve Sterbenz when he has problems in bringing the communities together to form program plans or reconcile differences. He might have some key people that he can count on to get the "flywheel" going.

APPENDICES

*Workshop on Defense, Basic, and Industrial Research
at the Los Alamos Neutron Science Center*

Appendix A:

Program

Workshop on Defense, Basic, and Industrial Research at the Los Alamos Neutron Science Center

Los Alamos National Laboratory J. Robert Oppenheimer Study Center
Rooms 216 and 218 February 12-15, 1995

Sunday Evening, February 12

6:00–8:00 pm Reception and Registration at the Bradbury Science Museum

Monday, February 13

8:00	J. C. Browne , <i>Director</i> <i>LANSCE and Energy Research Programs</i> <i>Los Alamos National Laboratory</i>	Registration, Welcome, Introductions, and Logistics
8:30	M. R. C. Greenwood , <i>Associate Director</i> <i>Office of Science and Technology Policy</i>	Science Policy in Changing Times
9:05	V. Reis , <i>Assistant Secretary</i> <i>Defense Programs, DOE</i>	Strategic Vision for DOE Defense Programs
9:40	I. Thomas , <i>Acting Associate Director</i> <i>Basic Energy Sciences,</i> <i>Office of Energy Research, DOE</i>	Plans for Future Neutron Facilities Within the DOE Office of Energy Research
10:15	Break	
10:30	S. S. Hecker , <i>Director</i> <i>Los Alamos National Laboratory</i>	Los Alamos National Laboratory Strategic Directions
11:05	J. Immele , <i>Director</i> <i>Nuclear Weapons Technology Programs</i> <i>Los Alamos National Laboratory</i>	Science-Based Stockpile Stewardship at Los Alamos National Laboratory
11:15	J. C. Browne , <i>Director</i> <i>LANSCE and Energy Research Programs</i> <i>Los Alamos National Laboratory</i>	Science-Based Stockpile Stewardship at LANSCE
11:30	R. Fortner , <i>Associate Director</i> <i>Physics and Space Technology</i> <i>Lawrence Livermore National Laboratory</i>	Why Does Livermore Need LANSCE?
11:45	D. Hayes , <i>Director</i> <i>Defense Programs Capabilities</i> <i>Sandia National Laboratories</i>	Lab Interdependencies and the Advanced Design and Production Technologies (ADaPT) Initiative
12:00	Panel Discussion and Audience Questions Theme: "Working Together" Chair, R. Pynn , <i>Deputy Director</i> <i>LANSCE & Energy Research Programs</i> <i>Los Alamos National Laboratory</i> Panel Members: Greenwood, Reis, Thomas, Hecker, Immele, Browne, Fortner, and Hayes	
12:45	Lunch	

2:15	A. K. Cheetham , <i>Director Materials Research Laboratory UC, Santa Barbara</i>	Neutron Scattering in Materials Research
2:50	G. Aeppli <i>AT&T Bell Labs</i>	Condensed Matter Research with Neutrons
3:25	Break	
3:40	S. Freedman <i>Dept. of Physics UC Berkeley</i>	Fundamental Physics with Neutrons
4:15	F. Dietrich <i>Physics and Space Technology Lawrence Livermore National Laboratory</i>	Nuclear Reaction Modeling, Verification Experiments and Applications
7:30–9:00	Report from Defense Science Breakout Session TA-3, SM-43, Room D356 (Weapons Meeting Room) (Q-clearance required)	

Tuesday, February 14

8:30	R. Pynn , <i>Deputy Director LANSCE & Energy Research Programs Los Alamos National Laboratory</i>	Existing & Planned Neutron Capabilities at Los Alamos National Laboratory
9:15	Breakout Sessions Start	
10:00	Break	
10:15	Breakout Sessions Continue	
12:00	Lunch	
1:00	Breakout Sessions Continue	
3:00	Break	
3:15	Breakout Sessions Continue	
6:00	Dinner at La Fonda, Santa Fe	

Wednesday, February 15

8:30	Breakout Sessions (<i>including drafting of report</i>)	
10:00	Break	
10:15	Breakout Sessions Continue	
12:00	Lunch	
1:00	Reports from each of the Breakout Groups	
3:00	Break	
3:15	Wrap-Up Discussions	

Breakout Sessions:

- MATERIALS SCIENCE AND ENGINEERING
Chair, T. M. Holden, AECL Chalk River Laboratories
- COMPLEX FLUIDS, POLYMERS, AND BIOSCIENCES
Chair, D. Schaefer, Sandia National Laboratories
- FUNDAMENTAL PHYSICS WITH NEUTRONS
Chair, G. Greene, National Institute of Standards and Technology
- APPLIED NUCLEAR PHYSICS
Chair, D. Strottman, Los Alamos National Laboratory
- CONDENSED MATTER PHYSICS AND CHEMISTRY
Chair, W. Nellis, Lawrence Livermore National Laboratory

Appendix B:

Participants

Workshop on Defense, Basic, and Industrial Research at the Los Alamos Neutron Science Center

Participant	Affiliation
Peter Adams	Los Alamos National Laboratory
Gabriel Aeppli	AT&T Bell Laboratories
Jim Anderson	Los Alamos National Laboratory
Bill Appleton	Oak Ridge National Laboratory
Edward Arthur	Los Alamos National Laboratory
Blaine Asay	Los Alamos National Laboratory
James Asay	Sandia National Laboratories
Ronald Atkins	Lawrence Livermore National Laboratory
John Axe	Brookhaven National Laboratory
Peter Barnes	Los Alamos National Laboratory
Walter Bauer	Sandia National Laboratories
John Becker	Lawrence Livermore National Laboratory
Stephen Becker	Los Alamos National Laboratory
Bard Bennett	Los Alamos National Laboratory
Tarlochan Bhatia	Los Alamos National Laboratory
Simon Billinge	Michigan State University
Alan Bishop	Los Alamos National Laboratory
W. P. Bishop	Department of Energy
J. Kent Blasie	University of Pennsylvania
Mark Bourke	Los Alamos National Laboratory
Thomas Bowles	Los Alamos National Laboratory
Charles Bowman	Los Alamos National Laboratory
David Bowman	Los Alamos National Laboratory
E. Morton Bradbury	Los Alamos National Laboratory
Karl Braithwaite	Los Alamos National Laboratory
Bruce Brown	Argonne National Laboratory
John Browne	Los Alamos National Laboratory
James Bryson	Sandia National Laboratories
Dick Burick	Los Alamos National Laboratory
Hugh Casey	Los Alamos National Laboratory
Mark Chadwick	Lawrence Livermore National Laboratory
Anthony Cheetham	University of California
Tom Claytor	Los Alamos National Laboratory
Donald Cobb	Los Alamos National Laboratory
Donald Cook	Sandia National Laboratories
Barbara Cort	Los Alamos National Laboratory
L. Scott Cram	Los Alamos National Laboratory
Mark Crawford	New Technology Week
Paul Cunningham	Los Alamos National Laboratory
Frank Cverna	Los Alamos National Laboratory
Jo Bart Czirr	Mission Support Inc.
Gregory D'Alessio	Department of Energy
Luke Daemen	Los Alamos National Laboratory
Robert Day	Los Alamos National Laboratory
Robert DeWitt	Department of Energy
Ram Devanathan	Los Alamos National Laboratory
Frank Dietrich	Lawrence Livermore National Laboratory
Paul Dotson	Los Alamos National Laboratory
Elliot Douglas	Los Alamos National Laboratory

Participant

Dawn Flicker
Richard Fortner
Stephanie Frankle
Stuart Freedman
David Funk
Alexander Gancarz
Avigdor Gavron
Michel Gerspacher
Paul Gilna
Damon Giovanielli
Terrence Goldman
Joyce Goldstone
Philip Goldstone
Geoffrey Greene
M.R.C. Greenwood

Patrick Griffin
E.C. Hagen
Earle Marie Hanson
Robert Hardekopf
Richard Harlow
Dennis Hayes
Sig Hecker
Mark Hedemann
Robert Henderson
Rex Hjelm
Earl Hoffman
Thomas Holden
John Hopson
Philip Howe
Steve Howe
Alan Hurd
John Immele
Jim Jackson
James Jorgensen
Raymond Juzaitis
Arthur Kerman
Nicholas King
Walt Kirchner
Rex Kiziah
Richard Krajcik
Michael Kreisler
George Kwei
Joseph Laia
A. C. Lawson
Paul Lisowski
Robert Little
Grant Logan
Terry Lowe
Ted Luera
John Lynn
Peter Lyons
Joe Mack

Affiliation

Los Alamos National Laboratory
Lawrence Livermore National Laboratory
Los Alamos National Laboratory
University of California
Los Alamos National Laboratory
Los Alamos National Laboratory
Los Alamos National Laboratory
Sid Richardson Carbon Co.
Los Alamos National Laboratory
Sumner Associates
Los Alamos National Laboratory
Los Alamos National Laboratory
Los Alamos National Laboratory
National Institute of Standards and Technology
Office of Science & Technology Policy
Executive Office of the President
Sandia National Laboratories
EG&G/EM
Los Alamos National Laboratory
Los Alamos National Laboratory
E. I. Dupont
Sandia National Laboratories
Los Alamos National Laboratory
Sandia National Laboratories
Los Alamos National Laboratory
Los Alamos National Laboratory
Los Alamos National Laboratory
Los Alamos National Laboratory
AECL Chalk River Laboratories
Los Alamos National Laboratory
Los Alamos National Laboratory
Los Alamos National Laboratory
Los Alamos National Laboratory
Sandia National Laboratories
Los Alamos National Laboratory
Los Alamos National Laboratory
Argonne National Laboratory
Los Alamos National Laboratory
Los Alamos National Laboratory
Los Alamos National Laboratory
Los Alamos National Laboratory
Pentagon
Los Alamos National Laboratory
Lawrence Livermore National Laboratory
Lawrence Livermore National Laboratory
Los Alamos National Laboratory
Los Alamos National Laboratory
Los Alamos National Laboratory
Los Alamos National Laboratory
Lawrence Livermore National Laboratory
Los Alamos National Laboratory
Sandia National Laboratories
Los Alamos National Laboratory
Los Alamos National Laboratory
Los Alamos National Laboratory

Participant

David Madland
Kim Mahin
Christian Mailhot
Charles Majkrzak
John Manning
Bruce Matthews
John McClelland
David McVey
Jas Mercer-Smith
Andre Michaudon
Pete Miller
Dennis Mitchell
David Moncton
George Morgan
Bruno Morosin
Chris Morris
Fred Mueller
Stephen Nayler
Tim Neal
William Nellis
Ron Nelson
Lawrence Newkirk
Cynthia Nitta
K. Henry O'Brien
Charles O'Farrell
Andy Obst
William Oosterhuis
Andrea Palounek
Seppo Penttila
Roger Perkins
Dave Phillips
Tom Picraux
Charles Prewitt
David Price
Roger Pynn
Jeffrey Quintenz
Partha Rangaswamy
Arthur Ratzel
Lauren Rauber
Victor Reis
James Rhyne
Thomas Rieker
Tony Rollett
Steve Rottler
Mike Rowe
Marie-Louise Saboungi
John Sarracino
Dale Schaefer
James Schirber
Stan Schriber
Lee Schroeder
Susan Seestrom
Robert Sheldon

Affiliation

Los Alamos National Laboratory
Sandia National Laboratories
Lawrence Livermore National Laboratory
National Institute of Standards and Technology
EG&G/EM
Los Alamos National Laboratory
Los Alamos National Laboratory
Sandia National Laboratories
Los Alamos National Laboratory
Los Alamos National Laboratory
Los Alamos National Laboratory
Sandia National Laboratories
Argonne National Laboratory
Los Alamos National Laboratory
Sandia National Laboratories
Los Alamos National Laboratory
Los Alamos National Laboratory
University of Florida
Los Alamos National Laboratory
Lawrence Livermore National Laboratory
Los Alamos National Laboratory
Lawrence Livermore National Laboratory
Lawrence Livermore National Laboratory
Lawrence Livermore National Laboratory
Sid Richardson Carbon Company
Los Alamos National Laboratory
Department of Energy
Los Alamos National Laboratory
Los Alamos National Laboratory
Los Alamos National Laboratory
Los Alamos National Laboratory
Sandia National Laboratories
Carnegie Institute of Washington
Argonne National Laboratory
Los Alamos National Laboratory
Sandia National Laboratories
Los Alamos National Laboratory
Sandia National Laboratories
Los Alamos National Laboratory
Department of Energy, Defense Programs
University of Missouri
Sandia National Laboratories
Los Alamos National Laboratory
Sandia National Laboratories
National Institute of Standards and Technology
Argonne National Laboratory
Los Alamos National Laboratory
Department of Energy
Sandia National Laboratories
Los Alamos National Laboratory
Lawrence Berkeley National Laboratory
Los Alamos National Laboratory
Los Alamos National Laboratory

Participant

Ning Shi
S. K. Sinha
Richard Slansky
Dennis Slaughter
Greg Smith
Johndale Solem
Walt Sommer
Constantine Stassis
Marion Stelts
Stephen Sterbenz
Michael Stevens
Barbara Stine
Galen Straub
Dan Strottman
Terry Taddeucci
Pier Tang
Iran Thomas
Kimberly Thomas
Robert Thomas
Joe Thompson
Richard Thompson
James Toevs
John Trabert
R. James Trainor
Walt Trela
James Tyler
John Ullmann
Olin VanDyck
Francesco Venneri
Robert Von Dreele
Gary Wall
Jerry Watson
Donald Weidner
Stephen Wender
H. R. Wenk
Paul Werner
Sam Werner
Geoffrey West
Roger White
Don Wolkerstorfer
Merri Wood
John Wooley
Steven Wright
Yi-Fen Yen
Phillip Young
Sandra Zink
Hans-Joachim Ziock
John Zumbro

Affiliation

Los Alamos National Laboratory
Exxon Research & Engineering
Los Alamos National Laboratory
Lawrence Livermore National Laboratory
Los Alamos National Laboratory
Los Alamos National Laboratory
Los Alamos National Laboratory
Ames Laboratory
Los Alamos National Laboratory
Los Alamos National Laboratory
Los Alamos National Laboratory
Los Alamos National Laboratory
Los Alamos National Laboratory
Los Alamos National Laboratory
Los Alamos National Laboratory
Department of Energy, Basic Energy Sciences
Los Alamos National Laboratory
Sandia National Laboratories
Los Alamos National Laboratory
EG&G/EM
Los Alamos National Laboratory
EG&G/EM
Los Alamos National Laboratory
Los Alamos National Laboratory
Lawrence Livermore National Laboratory
Los Alamos National Laboratory
Los Alamos National Laboratory
Los Alamos National Laboratory
Los Alamos National Laboratory
Los Alamos National Laboratory
Los Alamos National Laboratory
SUNY Stony Brook
Los Alamos National Laboratory
University of California, Berkeley
Sandia National Laboratories
University of Missouri
Los Alamos National Laboratory
Lawrence Livermore National Laboratory
Los Alamos National Laboratory
Los Alamos National Laboratory
Department of Energy, Health and Environment
Sandia National Laboratories
Los Alamos National Laboratory
Los Alamos National Laboratory
Los Alamos National Laboratory
Los Alamos National Laboratory
Los Alamos National Laboratory

Appendix C:

Abstracts from the Materials Science and Engineering Breakout Session

Computer Simulation of Radiation Effects in Materials

R. Devanathan, K.E. Sickafus, and M. Nastasi, Los Alamos National Laboratory

Abstract

Computer simulation can play a valuable role in improving our understanding of radiation damage processes in materials. The small time and distance scales, and the extremes of temperature and pressure that characterize the evolution of radiation damage make computer simulation an ideal tool for studying these processes. In addition, simulations enable us to isolate various defects and study their individual effects. The techniques commonly used to

simulate radiation damage are Monte Carlo, deterministic binary collision approximations, and molecular dynamics. The applicability of these techniques to a particular problem depends on factors such as the nature of the problem and the energy range of interest. The computer requirements, advantages, and drawbacks of these techniques will be discussed.

This research was sponsored by the U.S. Department of Energy, Office of Basic Energy Sciences, Department of Materials Sciences.

Characterization of Explosive Compacts

P. M. Howe, Los Alamos National Laboratory

Objectives

Composites of high explosives (HEs) and binders have structural aspects that reflect on the performance characteristics of the material. Important among these is HE particle size distribution, void size distribution in the HE, and the distribution of crack dimension between the binder and HE particles. The objective is to use neutron scattering techniques to measure each of these distributions in pristine HE composites and composites subjected to different process-related and accident-scenario-related procedures. This information will be used to provide parameters for simulations predicting the performance of the materials. Measurements on material performance would then provide essential information to validate and benchmark the simulations. The two principal advantages of using low-angle neutron scattering over other techniques are that it:

- is nonintrusive: no sample preparation is required, which is especially important for damaged explosives
- allows in-depth measurement, and eliminates surface preparation artifacts

Background

Numerous material parameters affect the response of an explosive to shock, impact, and thermal loading of the sort encountered in a variety of accident scenarios. In particular, the particle size distribution, the total porosity, and the pore size distribution are extremely influential in altering the sensitivity of explosives to shock loading. Small amounts of porosity significantly lower the pressure threshold required to initiate detonation. Shifts in the pore size distribution in an explosive markedly change the explosive response to shock and impact stimuli. Shifts in the particle size distribution or shifts in the crack size distribution can also have dramatic effects.

Generally, the larger the pores, the lower the ignition threshold, and the more sensitive the

charge becomes to impact and shock stimuli. While the presence of large pores lowers the ignition threshold, the presence of small pores accelerates burning and reduces the time to transit to detonation. Similarly, cracking and fragmentation of grains provides for accelerated burning. Generally, small particle sizes lead to more rapid transits to detonation. Similarly, cracking or fragmentation of particles accelerates burning.

Attempts to model the effects of these changes have been largely empirical. However, with the recent development of discrete element methods and other computational tools, we are attempting to model the phenomenology using the above as explicit input parameters.

In typical high-quality explosives used in nuclear weapons, the total porosity is reduced to a percent or less, and most of the very large voids are eliminated. Thus, in explosives designed for nuclear weapon use, the maximum pore size might be of the order of several microns, with the mean pore size being a small fraction of a micron. For explosives for conventional munitions, the mean and maximum pore size may be much larger.

In modern plastic bonded explosives (PBXs), a small amount of binder is included. Because the binder differs in shock impedance and in mechanical properties from the explosive, binder inclusions act in ways similar to voids, but less strongly. We are currently attempting to model the shock and flow interactions induced by binder inclusions. Currently, of course, we estimate the geometry and size distribution of the binder, as they are not directly measurable by standard techniques.

The porosity is easily determined from density measurements and knowing the theoretical maximum density. Currently, there is no direct way of accurately determining the pore size distribution. Standard metallographic techniques, such as cutting and polishing samples, are adequate for measuring particle size distri-

butions, but are inadequate for measuring pore size distributions because the softness of the materials causes the surface pores to be filled in polishing. Techniques such as BET adsorption or mercury porosimetry measure open pore sizes only. Open pores are a small fraction of the total porosity in design explosives.

The fragmentation of explosive grains as a result of compaction can be measured by various destructive means. For example, one can use ultrasonics to disassemble the compact and measure the fragment size directly. However, it would be far more useful to know the crack or fragment size distribution (and/or explosive surface area) in explosive samples which are then used in experiments. This provides a direct experimental correlation between the measured values and the explosive response.

The intergranular surface area is an extremely important parameter, as it strongly influences the nature of the post-ignition-burning reactions.

The following data are of immediate use:

- All our initiation models are based upon surface (or grain burning) models of one form or another. None of them explicitly use real data for surface area, and thus must be calibrated.
- We have developed a statistical crack mechanics model that describes the evolution of cracks with loading conditions, and predicts strain localization, fragmentation, heating, and ignition. As an input, the initial crack size distribution is required. We have no experimental data.
- We are using discrete element models and other computational techniques to model grain and binder interactions, frictional heating, ignition, burning, etc. We need experimental data against which to benchmark and test these models.

Proposed Experiments and Level of Effort

Characterization of Quasi-statically Compacted He

We propose to press molding powders of PBX 9501, PBX 9502, and PBX 9404 to different

final densities, using the procedures established for making weapons charges. Four different final densities for each explosive composition would be chosen, with five samples at each density. Portions of the samples will be ultrasonically disaggregated, and the resulting particle size and distributions and surface area measured directly for comparison with LANSCE results. Portions will also be subjected to burning rate measurements.

At LANSCE, each sample would be irradiated to determine the pore size distribution at density, the crack size distribution, the intergranular surface area, and the particle size distribution. Total porosity measurements will be made using gravimetric techniques before the LANSCE experiments.

The results will be used for direct comparison with material modeling of explosives and for comparison with reaction rate models.

Characterization of Damaged He

We propose to conduct five experiments with heavily confined explosive samples of PBX 9501. These samples will be impacted with flying plates at velocities below, but near, the reaction threshold. At LANSCE, the pore size distribution, crack size distribution, and particle size distribution of the samples will be measured as a function of velocity and as a function of distance from the point of impact. These data will be used to develop a spatial map of the above variable, and will be used for benchmarking models.

Characterization of Aged Materials

We have little data on the effects aging may have upon explosives. Aging in materials can be manifested in changes in the particle size distribution, changes in the internal crack distribution, changes in the binder bonding characteristics, and in directional grain growth. This latter effect may be especially important; experiments have shown that uniaxial pressing of explosives, as is done in a ram press, causes anisotropy in the explosive that significantly influences the detonation propagation characteristics (and, hence, warhead performance). We do not know yet how important these effects are in aged explosives. Each of the above

effects is somewhat amenable to investigation by various techniques. However, neutron scattering will provide information with respect to all of them and, when combined with analysis, will provide a very powerful means of assessing aged explosives.

Required Resources

The methodologies that need to be developed for this project are not new, but the application to a materials science problem is novel. Thus there is considerable development in-

volved. Further, the measurement of surface areas and dimension distributions will require developing computer codes and algorithms for data analysis. In addition there will be a requirement for designing and fabricating specialized instrument components for handling and mounting HE and HE composites.

Beam Time: One week each year

Points of Contact:

LANSCe: Rex Hjelm 505-665-2372

NWT: Philip M. Howe 505-665-5332

Proposed Budget

	Year 1	Year 2	Year 3
1.5 FTE TSM	\$360K	\$360K	\$360K
0.25 FTE Programmer	\$60K	\$10K	\$10K
0.15 FTE Technician	\$30K	\$30K	\$30K
Materials/Test Fixtures	\$60K	\$30K	\$25K
Total	\$510	\$430K	\$425K

Neutron Resonance Radiography Applied to Explosives Problems

P. M. Howe, Los Alamos National Laboratory

Background

Two major problems, which have historically been the bane of efforts in the explosives research, are addressable by neutron resonance radiography:

1. Qualitatively, it is known that microstructural effects in explosives strongly influence explosive sensitivity. An example of such a microstructural effect is hotspots in shock initiation. Hotspots are caused by the interaction of the shock wave with local density discontinuities such as voids and cracks or interfaces between explosive grains and binder. The interaction leads to very localized temperature excursions of hundreds of degrees Celsius. In explosives subjected to impact and deformation, other microstructural effects appear. Examples are shear cracking and shear banding. One of the major problems we face in the Explosives Technology Program is to develop accurate quantitative models which capture the contributions of the microstructure to explosives response. In particular, we need to extend our capabilities to measure and model the evolution of localized temperature excursions. We then use these results to describe their effect on the evolution of explosive reactions. We have a concerted experimental effort ongoing to measure the strain fields and temperature fields as a function of time in explosives subjected to moderate and high strain rates. These data will be used to guide and benchmark our modeling activities. All of our approaches employ either point measurements (as with thermocouples) or surface measurements (as with thermal imaging devices). Each of these techniques suffers from major difficulties. The optical approaches all have built in biases, and require assumptions that are not easily validated to generate quantitative measurements. (Pyrometry and infrared imaging both require assumptions about

the emissivity as a function of temperature and, in explosives, there are always questions about the location of the source radiation.) Fast response thermocouples would be ideal, but there are extreme experimental difficulties associated with thermocouple survival in materials undergoing high strain rate deformation and even more severe problems associated with their intrusive nature.

2. We have a long history of measurements of states achieved by shock loading materials (and by the detonation of explosives). Similarly, theoretical efforts to construct valid equations of state extend back over fifty years. State variables amenable to direct measurement are pressure, particle velocity, and shock velocity. From these measurements and initial state measurements, one can construct an incomplete equation of state. Direct (and accurate) measurements of temperature would allow constructing a complete equation of state. Conventional approaches to direct temperature measurement have been only partially successful. Thermocouples perturb the flow, usually have inadequate rise times for shock investigations, and have questionable calibrations. Pyrometry techniques have problems with the validity of underlying assumptions and with identification of the exact measurement region.

Approach

We plan to use neutron resonance radiography to make accurate temperature measurements in explosives under a variety of important experimental conditions. In each case, the approach involves use of a metallic dopant which has a very strong neutron resonance peak. The metallic compound is introduced in trace amounts (typically in the parts per million concentration) into the explosive in the region of interest. Since all our experiments involve explosives in reacting configurations,

the experiments will be used in small amounts, consistent with safe and prudent procedures. The resonance signal from the dopant is then measured by special detectors. The signal is then compared with a calibration matrix obtained from separate calibrations of signal shape versus temperature. The temperature is inferred from the Doppler broadening of the resonance peak.

Shear and Friction Experiments

For shear and frictional heating experiments, we will vapor deposit gold at the interface of interest. The low concentrations required permit its use without perturbing the material behavior. The experiments are designed to vary arbitrarily both applied pressure and sliding velocity. For a given set of sliding velocity and applied pressure, a series of experiments will be conducted with differing times of resonance sampling, so that temperature histories are generated for each velocity-pressure pair. Ten experiments per pair are planned. Experiments would be conducted with an explosive (PBX 9501) and its mechanical stimulant. Ancillary diagnostics include four color pyrometry and infrared imaging, which permit calibration of these latter diagnostics for further use in experiments at other locations.

Beam time: Two weeks, split into two-day segments.

Equations-of-State Experiments

Small cylinders of explosive will be detonated. The explosive of choice will have a small failure diameter (probably PBX 9501), so that steady propagating detonations can be obtained with confined charge diameters of less than a centimeter. The explosive will be doped with gold, which has a strong nuclear resonance signal. Consideration will be given to localizing the dopant to the center core of the explosive. This improves spatial resolution and eliminates wall effects. The explosive will be detonated and irradiated after passage of the detonation wave. Timing will be adjusted to permit sampling of the flow after detonation, but before the intrusion of strong rarefactions. Three different experimental configurations will be designed to provide temperature measurements in explosive products at markedly

different P-V-T states. The results will be compared with theoretical predictions.

Beam time: Two weeks

Multiple Temperature States

Porous materials subjected to rapid compression or shock loading develop multiple temperature states which slowly equilibrate. Measurement of the peak temperatures and the rate of equilibration is of strong theoretical and practical interest. This effort is designed to explore the possibility of making accurate measurements of both effects. Experiments will use porous compacts of differing particle size distributions. Initially, inert materials will be used. The porous compacts will be subjected to weak shock loading to generate significant temperature rises in both the matrix and at the sites of collapsing pores. At issue is whether or not sufficient resolution of the signal can be obtained in single burst experiments to permit accurate temperature definition. (Temperature assignment relies upon measurement of the peak width and shape. For materials with multiple temperatures, the peaks of differing shapes are superposed and must be deconvolved. As thermal equilibration occurs, the peaks will meld together. Accurate assignment of temperatures probably requires a discrete temperature distribution, i.e., one material fraction at one temperature, a second material at another temperature, with very little material at intermediate temperatures. As thermal equilibration occurs, the temperature gradients will become less steep and more and more material will be in intermediate states. This will cause signal blurring and melding, and aggravate difficulties in analysis.) The possibility of using two dopants will be considered; one which pervades the solid material, the other as a coating of the particles. Thus, the coating will see predominately the temperatures associated with hotspots, the bulk dopant will see predominately temperatures of the bulk. A series of fifteen exploratory experiments using inerts is planned. Five experiments using porous explosive compacts are planned.

Beam time: Two weeks, split into two-day segments.

Calibration of Conventional Techniques

The use of neutron radiography for temperature measurements has major advantages over other techniques available to the explosives research community. However, it has the disadvantages of low availability of beam time and lack of flexibility for explosives experiments. Thus, we need to continue the development and application of other temperature measurement techniques for use at our regular

experimental sites. However, the neutron resonance radiography technique can significantly enhance these other methods by providing accurate and precise calibrations. We thus plan a series of ten experiments (two different experimental configurations, five temperature states each) to calibrate our multi-color pyrometry and infrared imaging systems.

Beam time: One week, in two-day segments.

Proposed Budget

Required Resources (\$K)	Year 1	Year 2	Year 3	Year 4
LANSCE				
1 FTE TSM	240	240	240	240
1 Postdoc	60	60	60	60
Beam Time as above				
NWT				
1 FTE TSM	240	240	240	240
1 FTE Technician	200	200	200	200
Materials/Fixtures.	100	75	50	50
Computer Support	25	25	25	25
Programming Support	30	30	30	30
Total	895	870	845	845

Characterization of Stockpile Materials at LANSCE

L. R. Newkirk, Lawrence Livermore National Laboratory

The Livermore program for stockpile materials characterization to be executed at LANSCE currently has three major components: residual stresses in welds, bonds, and joints; texture development in new fabrication processes; and analysis and prediction of sensitivity in high explosives. Execution of these projects relies on the application of neutron diffraction, inelastic neutron scattering, and small-angle scattering.

Residual Stresses

We have considered three problems of interest in stockpile stewardship, two of which are very specific and the third more generic. The application of neutron diffraction to these problems takes advantage of the penetration of neutrons to measure bulk properties. The first of these, and the one we will begin addressing with experiments this summer, is the measurement of stress in silver interlayer bonds. It has been established that the aging behavior of these bonds is strongly influenced by the stress in the bond. However, the stress in this unusual geometry must be calculated by finite element methods with no direct experimental confirmation or validation. The initial measurements will be carried out on a surrogate system utilizing a silver alloy braze of comparable thickness to the diffusion bond, or possibly an actual diffusion bond, joining two pieces of maraging steel. These measurements will establish the feasibility of extracting the required strain data from the small volume of the bond. The other two areas of interest, which will not be undertaken immediately, are the characterization of strain in a beryllium joint and the more generic issue of providing

experimental data to improve modeling of residual strain in a variety of welds.

Texture

We plan to use the neutron diffraction equivalent of an x-ray pole figure to obtain bulk measurements of crystallographic texturing in uranium alloys during fabrication by spin-forming. This will complement an ongoing effort to develop constitutive data for this system at large strains to enable improved finite element modeling of the fabrication process. While similar data could be obtained from either x-rays or backscattered electrons (Kikuchi pattern), such measurements would be extremely surface sensitive. Extremely tedious and careful metallographic preparation would have to be carried out repeatedly to avoid being misled.

High-Explosive Sensitivity

Our initial focus in addressing high-explosive sensitivity will be the use of inelastic neutron scattering to characterize the phonon spectra in high explosives. We have evidence from extensive molecular dynamic calculations suggesting a strong correlation between the experimentally measured sensitivity using the drop-hammer technique and the efficiency of phonon to vibron up-conversion at specific wave numbers. It is important that we experimentally examine this mechanism to understand and validate its importance. Although this is only one aspect of explosive sensitivity, it will permit us to better predict explosive behavior as well as enhance our ability to search for new insensitive high explosives.

Appendix D:

Abstracts from the Applied Nuclear Physics Breakout Session

Experimental Measurements Supporting the Advanced Fission Model

*J. B. Becker and E. A. Henry, Lawrence Livermore National Laboratory
R. Nelson and S. Wender, Los Alamos National Laboratory*

The Advanced Fission Model proposed by D. Madland requires detailed measurement of

- the cross section for fission as a function of incident neutron energy
- detailed mapping of the fission products, including
 - a) the isotopic identification of the fragments
 - b) energy spectrum of emitted neutrons $N(E)dE_n$
 - c) kinetic energy of fragments $E_x(f)$

The combination of LANSCE and a large-scale detector array facilitates measurements of all these quantities excluding the fragment kinetic energies; these can, however, be estimated if the detector array also has the capability of neutron measurement. A multidetector array with large resolving power for gamma-ray detection is the key component because mapping the Z,A and excitation of each fission fragment requires coincidence of gamma-ray measurements of the correlated fragment pairs.

LANSCE offers the required white neutron source but does not have a large-scale array for gamma-ray, x-ray, and neutron detection. A new array could be constructed at a cost of 2-

to 3-million dollars over 2 years. Efforts are being made to bring a large-scale gamma-ray array (HERA) to LANSCE. HERA is available because the GAMMASPHERE project has been developed at the Lawrence Berkeley National Laboratory (LBNL) 88-Inch Cyclotron. HERA is one of three large-scale arrays in the U.S. A proposal has been made to LBNL/DOE (Energy Research) to site HERA at LANSCE. All detectors, electronics, and a data acquisition computer was included in the request. Funding was not included in that proposal. It is approximately a 4 FTE \times 4-month job to have HERA operational on an existing site with utilities at LANSCE and WNR.

Gamma-ray spectroscopy is fundamental to experimental neutron science. The white source of LANSCE coupled with a large-scale gamma-ray detector array is a unique powerful combination for neutron science. This combination is the preferred tool to meet many nuclear data requirements, including the Advanced Fission Model, (n,xn) cross sections on ^{239}Pu and other elements mentioned in this session, and data requirements we have not yet anticipated. Finally, this combination impacts all neutron science and ensures a leadership role for the Los Alamos Neutron Science Center.

Advanced Post-Scission Fission Model

D. G. Madland, Los Alamos National Laboratory

The neutrons coming from the de-excitation of fission fragments constitute the major portion of the neutron spectrum of any modern nuclear reactor system. These neutrons burn the reactor fuel. They are emitted in competition with gamma rays from the de-excitation of the two fission fragments occurring in binary fission (approximately 1 in 400 fissions is ternary). The kinetic energies of the two fission fragments make up the major portion of the energy release in fission and therefore the major portion of the thermal energy in the reactor. The fission-fragment yields, the neutrons and gamma rays (multiplicities and spectra) coming from fission-fragment de-excitation, and the fission-fragment kinetic energies are examples of post-scission fission observables, that is, physical observables appearing after the snapping of the neck between the two nascent fission fragments making up the compound fissioning nucleus.

Almost all of the post-scission fission observables are, in fact, distributions: for example,

- approximately 500 fission fragment species occur
- neutron and gamma-ray multiplicities change with fission-fragment species
- fission-fragment kinetic energies change with fragment mass
- prompt fission neutron spectra change with incident neutron energy

However, many of the present reactor design codes contain only *average* values for these distributions, for example, the average total fission-fragment kinetic energy, the average prompt fission neutron multiplicity (as a function of the energy of the neutron inducing fission), average fission fragments and their corresponding neutron cross sections, and an average prompt fission neutron spectrum. The essence of the Advanced Fission Model is to

replace *average values* of post-scission observables by the *distributions* of these observables together with their *correlations*.

The Advanced Post-Scission Fission Model can be constructed in the following steps:

1. Use experimental fission-fragment mass and charge distributions when they exist and otherwise multiple-Gaussian (5 or 7) and Gaussian approximations, respectively. This will involve physically-based parameterizations of the Gaussian approximations.
2. Use experimental fission-fragment kinetic-energy distributions when they exist and otherwise multiple-Gaussian (perhaps 2 or 3) approximations with physically-based parameterizations.
3. Install a Hauser-Feshbach statistical-model code in a driver that loops over the fission-fragment mass, charge, and kinetic-energy distributions for, say, a given incident neutron energy and performs the appropriate summations for the specific observables desired.
4. Determine a global neutron optical model potential with a physically realistic dependence (fission-fragment nuclei have relatively large isospin and are sufficiently far from the β -stable line that few elastic neutron scattering data exist) for use in the Hauser-Feshbach code.

Within this framework essentially all of the post-scission fission observables can be calculated as functions of the fission-fragment yield and/or fission-fragment kinetic energy and/or incident neutron energy and/or integrals over these quantities.

Reaction Theory Calculations to 200 MeV for Applications*

*P. G. Young, Los Alamos National Laboratory
M. B. Chadwick, Lawrence Livermore National Laboratory*

Summary

The possibilities of several new technologies based on the use of intense, medium-energy proton accelerators are being investigated at Los Alamos National Laboratory (LANL). The potential new areas include destruction of long-lived components of nuclear waste, plutonium burning, energy production, and production of tritium. The design, assessment, and safety analysis of potential facilities involves the understanding of complex combinations of nuclear processes, which in turn places new requirements on nuclear data that transcend the traditional needs of the fission and fusion reactor communities. Additionally, other areas of technology such as neutron and proton therapy applications, which are being developed at Lawrence Livermore National Laboratory (LLNL), are also placing new requirements on nuclear data.

The LAHET Code System (LCS) has been developed at Los Alamos to perform comprehensive neutronics and radiation analyses of nuclear systems that involve particle energies greater than 20 MeV, which is currently the energy limit for neutron reactions in the U.S. national nuclear data system, ENDF/B. At present, an intranuclear cascade plus evaporation model is used in the LAHET code to calculate nuclear data for all neutron interactions occurring at energies greater than 20 MeV, and for charged-particle reactions at all energies down to a lower energy cutoff. Use of the intranuclear cascade model at energies below ~150 MeV is known to be inappropriate, particularly for lighter elements, and this procedure is followed primarily because of the unavailability of reliable evaluated libraries at energies above 20 MeV. A collaborative effort involving personnel from N-Division at LLNL and X- and T-Divisions at LANL is planned to improve the nuclear physics information, particle transport capability, and overall reliability of the nuclear analysis code system at Los Alamos.

In this paper, the importance of developing neutron and proton cross section libraries in the incident particle energy range of 20 MeV to approximately 200 MeV for transport applications is discussed, and new theoretical methods for developing cross section libraries at higher neutron and proton energies are summarized. We have made a number of modifications to the nuclear model code GNASH in order to improve the accuracy of calculations at incident particle energies up to 200 MeV. Most important among the changes is the adaptation of the code to permit its use in conjunction with quantum mechanical preequilibrium calculations, the so called FKK-GNASH version of the code. We have also incorporated a model for calculating multiple preequilibrium effects, that is, we permit particle-hole states formed after the first preequilibrium particle is emitted to further decay by "multiple preequilibrium" emission. Additionally, we have incorporated models for estimating spin distributions of preequilibrium contributions using angular momentum distributions based on the exciton model, and for improving the excitation energy dependence of the particle-hole state densities used in the exciton model calculations.

In this presentation, we illustrate the significance of the model improvements and include comparisons of calculations with experimental data for several target materials that are important in applications. In particular, we show results for calculations with both GNASH and FKK-GNASH of (p, xn) and (p, xp) reactions for 160-MeV protons on ^{90}Zr and ^{208}Pb , allowing a comparison of semiclassical and quantum descriptions of preequilibrium emission for high energies. We illustrate how the code system can be most effectively utilized for higher energy analyses. We also investigate angular momentum effects in our equilibrium and preequilibrium modeling by analyzing phenomena sensitive to spin distributions: high-resolution measurements of $(n, xn\gamma)$ discrete gamma-ray production for incident neutron

energies to 200 MeV. Finally, we describe how such measurements can be combined with theoretical calculations to obtain (n,xn) cross

section information needed for defense and other applications that is otherwise sparse or unavailable.

Appendix E:

Abstracts from the Condensed Matter Physics and Chemistry Breakout Session

Fine-Scale Texture in Complex Electronic Materials

A. Bishop, Los Alamos National Laboratory

We are faced with a new paradigm in modern condensed matter science (soft-condensed matter, complex-electronic materials). Namely, how is the macroscopic functionality (electronic, optical, magnetic, strength) controlled by *intrinsic* inhomogeneities—"texture" on multiple and hierarchical fine scales (in space and time).

This is the "mesoscopic" domain between microscopic and macroscopic descriptions and is beyond traditional materials science descriptions of texture scales (domains, grains, etc.). Intrinsic fine-scale texture refers to precursor structures, long-period (superlattice) order, polaronic distortions, etc. that are the result of intrinsically coupled (and often competing microscopic interactions—spin, charge, and lattice. Relevant classes of materials include: perovskite ferroelectrics, high T_c superconductors, mixed-valence colossal magnetoresistance materials; Martensitic, elastic, and shape-memory alloys (including plutonium, its aging and microstructural response to external perturbations); self-assembling polymers and macromolecular heterostructures; etc.

To probe the coupled electronic and structural aspects of the fine-scale structure on the appropriate multiple space- and time-scales requires *new* resolutions and *combinations* of experiments—neutron, x-rays, XAFS, NMR, ion-channeling, etc. The very recent time-of-flight data now emerging from spallation neutron sources (in the case of "phonons," from ISIS—MARI) have already revolutionized the *local* structural information in high- T_c superconductors. Pair-distribution-function analysis, and energy-resolved pair-distribution-function analysis (not simply in liquids but complex unit cell solids) are set to become major new tools for the suite of experimental techniques we need to assemble—not just for high T_c superconductors, but *all* of the classes of material mentioned above.

The notion of "synthesis/processing-structure-property" relationships has key underpinning science issues that we now have the opportunity (and need to address). Accelerator-based neutrons are an essential element of understanding and controlling this science.

Direct Observation of Short-Range Order in Complex Materials

S. J. L. Billinge, Michigan State University

Neutron diffraction has been immensely successful at solving the crystal structures of materials. However, the problem of solving the local arrangements of atoms in disordered materials, or in materials with a disordered component to the structure, has proven to be much more difficult. A variety of techniques, such as nuclear magnetic resonance, x-ray absorption fine structure analysis, and Mössbauer spectroscopy, now are available for studying this problem.

In this talk, I described the use of neutron powder diffraction data to obtain short and intermediate range, structural information from complex materials. The technique is called pair distribution function (PDF) analysis and relies on the fact that the real-space atom-pair correlation function, which describes the internal arrangement of atoms in a solid, is the direct Fourier transform of the experimentally recovered diffraction pattern from a powder sample. Thus, by carefully collecting powder diffraction data over a wide range of Q (Q is the magnitude of the scattering vector), making suitable corrections to the data, and then Fourier transforming it, it is now possible to obtain highly accurate PDFs from real materials.

This type of analysis is clearly important in understanding the fundamental properties of complex materials since it yields, quantitatively, local structure parameters which can dictate the properties of the material. I foresee that close collaborations will develop among computational physicists and chemists and people involved in these measurements who attempt not only to *model* the local structures but to understand their origin (electron-lattice interactions for example) and their impact on the properties of materials. Such an understanding can also lead to improved materials design and synthesis. In addition, because the atomic structure can be probed as a function of length in the material,

the possibility exists of crossing over into the realm of microstructure and studying domain structures and extended defects such as interfaces from the local structure point of view. This could yield information, for example, about the energetics of these defects due to local strains, or, for example, help to elucidate the microscopic origin of precursor microstructures such as tweed, which is seen in a number of technologically interesting materials such as martensitic shape-memory alloys and high-temperature superconductors.

The success of these measurements depends in large part on the availability of large fluxes of high-energy neutrons. Time-of-flight measurements made at spallation sources are the ideal method of collecting data, yielding high quality data in a relatively short time over wide regions of Q -space. Successful measurements have already been made at LANSCE (using the HIPD diffractometer) and at IPNS (using SEPD). HIPD has the advantage of a large flux which allows data to be collected with good precision in a relatively short time period; on the other hand, SEPD yields data with better resolution, yet still with adequate flux. Right now the capability of the technique is being developed. Within a few years, we expect that the technique will be ready to be applied to a large number of problems in the physics, chemistry, and materials science of complex materials.

The continued availability of powder diffractometers like SEPD and HIPD, and the development of new instruments such as GLAD (at Argonne) and other powder diffractometers optimized for this kind of measurement, will be very important for the success of this endeavor. It should be noted that the existing powder diffractometers at pulsed sources are already oversubscribed and the expanded demand for their use will put severe pressure on the system.

Resolving Local Structures on Different Time-Scales Using Neutron Powder Diffraction

S. J. L. Billinge, Michigan State University

In a kinematical scattering experiment such as neutron diffraction, the time-scale of the experiment depends on the energy resolution of the measurement. Thus, in principle, it is possible to vary the time-scale on which you probe the structure by systematically varying the energy resolution. This is possible using pulsed neutrons by explicitly measuring the dynamical structure factor, $S(Q, w)$, over a wide range of Q and w (where Q is the magnitude of the scattering vector and hw is the energy transfer) and integrating over w in a controlled way, as we describe below. This capability is important when studying phenomena such as phase transitions, the glass transition, and any dynamical property of the lattice where the structure you see depends on how fast you probe the lattice.

Using pulsed neutrons it is possible to *survey* a wide range of (Q, w) space at one time using a chopper spectrometer, yielding both elastic and inelastic scattering explicitly. These data are suitable for Fourier transforming into real-space to obtain the pair distribution function (PDF) of the material. By Fourier transforming just the elastic ($w = 0$) line you recover the time averaged structure. However, after integrating over w at constant Q for each Q -point, you recover the total structure factor, $S(Q)$, which yields the instantaneous local structure in the PDF. In principal, all time-scales between these extremes are accessible by sys-

tematically varying the range of integration of the w not = 0 scattering. *Thus, by combining the energy resolved scattering and the PDF technique it is possible to resolve the structure over a wide range of length and time scales.*

The technology exists to do this. Preliminary measurements have been made using the MARI spectrometer at ISIS in the UK by Profs. Arai and Egami. However, the Q resolution of MARI is marginal for this measurement and more development work is required before reliable results can be demonstrated. This is extremely difficult because MARI is heavily oversubscribed and it is impossible to obtain adequate beam-time to do this experiment, especially for U.S. scientists who do not have priority at this European-Japanese facility. The proposed Phase II development of the PHAROS spectrometer at LANSCE, which involves installing wide-angle detector banks into this fast chopper spectrometer, will yield a machine with superior Q -resolution to MARI, which can access the wide range of (Q, w) space necessary for these measurements. This will make it the primary facility in the world for this kind of measurement and allow adequate access to do the necessary developmental work to realize the full potential power of this technique. *The completion of Phase II of the PHAROS spectrometer construction is essential if this research is to succeed.*

DuPont's Use of Neutron Facilities

R. Harlow, E. I. Dupont

From 1991 to 1995

Neutron powder diffraction has played a major role in understanding the changes in the structure and properties of the La_2CuO_4 family of superconductors as a function of doping.^{1,3,5} The general formula of the compounds which have been studied can be represented as $\text{La}_{1-x-y}\text{Re}_x(\text{Sr},\text{Ba})_y\text{CuO}_{4+\delta}$, where Re is any number of smaller rare earth elements including Nd, Sm, Gd, and Dy. This La_2CuO_4 family has been shown to undergo a number of phase transitions at lower temperatures caused by various tilts of the CuO_6 -octahedra. These tilts occur in both the Sr and Ba superconductors, and can generally be increased in magnitude by the additional substitution of smaller rare-earth ions. It has been shown that these tilts have adverse effects on T_c . Extra oxygen in the lattice seems to inhibit these tilts but these compounds has not been fully studied. 1/8-hole doping also has a dramatically negative affect on T_c but it has now been clearly demonstrated that it not structural in origin. This study of the Cu superconductors has lately been extended to include the chemically simple but structurally complex strontium copper oxides¹¹ and, most recently, the strontium analogs of the 123 family of superconductors.¹³

There are a number of compounds which have nearly the same structure as La_2CuO_4 and, in some cases, these even have the same 1/2-spin on the transition metal ion. Of particular interest have been the Sr_2MO_4 family, where $M = \text{Ir}, \text{Ru}, \text{Rh}, \text{V}, \text{and Ti}$.^{6,8} Of these, only the Ru compound is known to superconduct with a T_c of approximately 1 K. Our initial focus, however, was on the Ir (spin = 1/2) compound which, from very careful synchrotron and neutron powder experiments, showed superlattice peaks indicative of a rotational distortion of the IrO_6 octahedra. Still unanswered is the question: why does the CuO_6 octahedra in La_2CuO_4 distort by tilting and the IrO_6 octahedra distort by rotation? The Rh compound also distorts by rotation, but Ru, V, and Ti compounds do not distort at all even though

there is just as much interlayer stress in these as in the Rh and Ir compounds. The Ti compound has no unpaired electrons but the V and Ru compounds clearly do. We are continuing our studies into the magnetic and electronic properties which distinguish these compounds from La_2CuO_4 .

Neutron powder diffraction has also been used to refine the crystal structures of several new phases of aluminum fluoride as part of program to find new catalysts for the production of chlorofluorocarbon alternatives.¹⁰ These new AlF_3 phases were made by careful thermal decomposition of various "organic" aluminum fluorides and, thus, only existed as microcrystalline powders. The structures of these compounds were initially solved *ab initio* from their synchrotron powder diffraction patterns but were refined using both the x-ray and neutron powder data. One of these new phases has shown some promising catalytic activity. Other studies related catalysis include the refinement of the structures of a novel open-framework structure,² prompt-gamma analysis of acid sites in solid superacids,⁹ and the determination of host-guest interactions on the conformations of hydrofluorocarbons adsorbed in zeolites using inelastic neutron scattering techniques.¹²

A number of x-ray crystal structures have been done to support the notion that imidazol-2-ylidene compounds are true carbenes containing a carbon atom which forms only two bonds with neighboring atoms and has two non-bonding electrons. These structures give evidence to the fact that the carbon is bonded to only two neighbors but cannot prove the existence of the non-bonded electrons. By using a combination of neutron (scattering from the nuclei) and x-ray (scattering from the electrons) single-crystal diffraction, it has been possible to map out the valence electron density of one of these carbene molecules.⁷ The map which results clearly demonstrates the presence of the carbene electrons in complete

agreement with the position predicted from quantum-mechanical calculations.

A fair amount of work on polymers has been done by DuPont personnel but only a small portion of it has, as yet, been published. Wide-angle neutron diffraction has been used to study copolymer segregation as part of a wider program to develop structure/property relationships in polymers.⁴ Other polymer studies have used small-angle scattering to characterize the formation of micelles and laminar morphologies in semi-crystalline polymers and polymer blends. Reflectivity measurements have been used to study polymer interdiffusion across interfaces and exchange dynamics from solid surfaces of polymers.

Future Usage

In the past, much of our interactions with the neutron facilities has been driven by projects with a great deal of "personal" and scientific interest. Given the present trend to focus more on projects relevant to the company's business units, it is highly probable that the superconductivity effort, in particular, will diminish. Interest in powder diffraction will, however, continue to be used to refine novel structures, particularly structures related to the catalysis program. The much-abused term "in situ" will become more meaningful as the need to study heterogeneous catalysts under real (2000 psi, 350°C) operating conditions becomes a reality. To run a successful catalyst program, the user facilities should be prepared to accommodate a large quantity of chemical apparatus and methods to deal with a number of potential chemical hazards. The use of prompt-gamma and inelastic neutron scattering also hold a great deal of promise for catalyst studies. Hereto, the most informative studies would be those of an "in situ" nature.

Fundamental scientific studies of the type exemplified by the X-N valence-density study noted above will probably not be encouraged in the future. Neutron, single-crystal structural studies will need to made more routine (smaller crystals, higher fluxes, better detectors) if companies like DuPont are ever to take real advantage of them.

Studies of polymer systems, especially those designed to complement our synchrotron studies, could benefit from DuPont's emphasis on its core polymer businesses. The investigation of these structural complex systems require a multitechnique approach and the advantages of neutrons are well known. Real-time, simultaneous small- and wide-angle diffraction studies could prove to be very popular.

Interest is growing in the structures of poorly crystalline and amorphous materials. We are presently developing our capabilities to convert x-ray (synchrotron) powder diffraction patterns automatically into pair-distribution functions. It is clear that the information that we are obtaining could be greatly augmented by similar conversions of neutron powder diffraction patterns. Tomography is another possible growth area; we have received a number of requests to look at manufactured products in order to look for defects.

References

1. M. K. Crawford, R. L. Harlow, E. M. McCarron, W. E. Farneth, J. D. Axe, H. Chou, and Q. Huang, "Lattice Instabilities and the Effect of Copper Oxygen Sheet Distortions on Superconductivity in Doped La_2CuO_4 ," *Phys. Rev B* **44**, 1749 (1991). NIST, HFBR
2. J. B. Parise, D. R. Corbin, T. E. Gier, R. L. Harlow, L. Abrams, and R. B. Von Dreele, "Flexibility of the RHO Framework: A Comparison of the Rb-exchanged Zeolite and the Novel Composition $\text{Rb}_{24}\text{Be}_{24}\text{As}_{24}\text{O}_{96} \cdot 3.2\text{D}_2\text{O}$," *Zeolites*, **12** 360-368 (1992). LANSCE
3. M. K. Crawford, W. E. Farneth, R. L. Harlow, E. M. McCarron, R. Miao, C. C. Torardi, J. D. Axe, H. Chou, and Q. Huang, "Structural Phase Transitions in Insulating and Metallic La_2CuO_4 ," in *Proceedings of the Workshop on Lattice Effects in High- T_c Superconductivity*, Santa Fe, Jan. 13-15, 1992, Y. Bar-Yam, T. Egami, J. Mustre-de Leon, and A. Bishop, Eds. (World Scientific Publishing, 1992). NIST, HFBR

4. K. H. Gardner, B. S. Hsiao, and K. L. Faron, "Neutron Study of Selectively Deuterated Poly(aryl ether ketones)," *Proceedings of the American Chemical Society* **67**, 216–217 (1992). NIST
5. M. K. Crawford, R. L. Harlow, E. M. McCarron, W. E. Farneth, N. Herron, H. Chou, and D. E. Cox, "Structural Phase Transitions and Interlayer Magnetic Interactions in $\text{La}_{2-x}\text{Nd}_x\text{CuO}_{4+\delta}$," *Phys. Rev. B* **47**, 11623–11626 (1993). HFBR
6. M. K. Crawford, M. A. Subramanian, R. L. Harlow, J. A. Fernandez-Baca, Z. R. Wang, and D. C. Johnston, "Structural and Magnetic Studies of Sr_2IrO_4 ," *Phys. Rev. B* **49**, 9198–9201 (1994). HFIR
7. A. J. Arduengo, III, H. V. R. Dias, D. A. Dixon, R. L. Harlow, W. T. Klooster, and T. F. Koetzle, "Electron Distribution in a Stable Carbene," *J. Amer. Chem. Soc.*, 6812–6822 (1994). HFBR
8. M. A. Subramanian, M. K. Crawford, R. L. Harlow, T. Ami, J. A. Fernandez-Baca, Z. R. Wang, and D. C. Johnston, " Sr_2RhO_4 and Sr_2IrO_4 : Structural and Magnetic Studies of 4d and 5d transition metal analogs of La_2CuO_4 ," *Physica C* **235–240**, 743–744 (1994). HFIR
9. M. K. Crawford, D. R. Corbin, and P. D. VerNooy, "Prompt Gamma Activation Analysis of Solid Acid Catalysts," *Transactions of the American Nuclear Society* **71**, 168–169 (1994). NIST
10. N. Herron, D. L. Thorn, R. L. Harlow, G. A. Jones, J. B. Parise, J. A. Fernandez-Baca, and T. Vogt, "The Preparation and Structural Characterization of Two New Phases of Aluminum Trifluoride," *Chem. of Materials* **7**, 75–83 (1995). HFIR, HFBR
11. T. Ami, M. K. Crawford, R. L. Harlow, Z. Wang, D. C. Johnston, Q. Huang, and R. C. Erwin, "Magnetic Susceptibility and Low Temperature Structure of the Linear Chain Cuprate Sr_2CuO_3 ," *Phys. Rev. B*, accepted. NIST
12. T. J. Udovic, J. M. Nicol, R. R. Cavanagh, J. J. Rush, M. K. Crawford, C. P. Grey, and D. R. Corbin, "Neutron and Raman Spectroscopies of 134 and 134a Hydrofluorocarbons Engaged in Na-X Zeolite," *Proceedings of MRS Symposium on Neutron Scattering*, Boston, accepted. NIST
13. M. A. Subramanian, R. L. Harlow, G. H. Kwei, and R. Suryanarayana, "Single Crystal X-ray and Powder Neutron Diffraction Studies of Dopant Site Preference and Oxygen Defect Structure in $\text{YSr}_2\text{Cu}_{3-x}\text{MxO}_{7+\delta}$ ($\text{M} = \text{Mo}, \text{W}, \text{and Re}$)," in progress. LANSCE

Advanced Materials Research Using a Pulsed-Spallation Neutron Source

J. Jorgensen, Argonne National Laboratory

Powder diffraction at a pulsed-spallation neutron source can play a central role in any advanced materials research program. The comprehensive work on high- T_c oxide superconductors over the last 8 years provides a useful benchmark of what performance can be expected. The LANSCE facility when operation at 80- μ A beam current (assuming equivalent instrumentation) will achieve performance neutron count rates about five times that of the IPNS facility, on which most the performance estimates are based. Estimates of expected performance can be made in the following areas.

Structure Refinement from Powder Data

With modern Rietveld techniques, accurate structural information (e.g., atom positions, site occupancies, etc.) can readily be obtained from powder neutron diffraction data. The most common use is to probe structural properties versus changes in composition or external conditions (e.g., temperature, pressure, etc.). A typical sample can be run on 2 to 4 hours, allowing hundreds of samples to be run over an extended period of time. In fact, with an in-house neutron facility available, neutron powder diffraction becomes an important analytic tool, used much in the same way as x-ray diffraction is used in most laboratories.

High Temperature, Including Controlled Atmospheres

Data collection at a temperature above or below room temperature is routine at most neutron facilities. The ability to collect data at high temperature has been particularly useful for work on the oxide superconductors for two reasons. First, measurements of the response of the structures to changes in temperature, while controlling the oxygen atmosphere seen by the sample, were the key to understanding how oxygen content controlled the properties of these compounds. Second, there have been

a number of *in situ* neutron diffraction studies of reaction chemistry, which provide important information about the reaction kinetics and intermediate phases in the reaction process. For these compounds, experimental conditions have been in the range of 10 to 1400 K with oxygen partial pressures of 10^{-6} -1 atm.

High Pressure

The time-of-flight techniques used at a pulsed neutron source are advantageous for data collection at high pressure because of the ability to collect data at a single, fixed scattering angle. For the oxide superconductors, high pressure was used to explore the relationship between structure and superconducting properties because it allows a way to vary the structure without changing the composition. In a more general context, it is often important to investigate phases or phenomena that occur only at elevated pressure or to probe the properties of materials at the pressures they will encounter in their working environments. For the oxide superconductors, pressures to 6 kbar in hydrostatic helium gas systems and to 150 kbar in quasi-hydrostatic conditions using an opposed anvil cell were used.

Realtime Phenomena

The rapid data collection that is possible on present pulsed neutron sources allows the study of kinetic phenomena in real time. For the oxide superconductors, this included the study of diffusion-limited processes, ordering phenomena (that were found to have a profound effect of superconducting properties even though the ordering takes place on a short-length scale), and reaction chemistry. Data of sufficient quality for full Rietveld refinements (providing atoms' positions or site occupancies) were obtained in time windows as short as 5 minutes. Time windows as short as 1 minute should be possible at LANSCE.

Small Samples

It is often the case that only small samples are available for study because of the expense or difficulty of making the samples. For the high- T_c oxide superconductors, this was the case for samples made by high-pressure techniques. By minimizing backgrounds, it has been possible

to obtain useful diffraction data (suitable for Rietveld refinement) from samples as small as 20 mg using the Special Environment Powder Diffractometer at IPNS. The study of even smaller samples should be possible at LANSCE with proper attention to instrument backgrounds and sample mounting techniques.

Goals for Science-Based Stockpile Stewardship at LANSCE

A. C. Lawson, Los Alamos National Laboratory

LANSCE should contribute to science-based stockpile stewardship by providing data that improve the scientific understanding of materials used in the nuclear weapons stockpile.

- Debye-Waller factors of the actinides and other materials

LANSCE should be used to measure Debye-Waller temperatures (a thermal measure of the elastic constant) and their temperature dependence. This is a poor man's road to equation-of-state data, as single crystals are not required.

- Phase characterization of materials

Neutron diffraction and small-angle scattering at LANSCE should be used to characterize materials for fire-resistant, surrogate, and other applications.

- Phonon spectra of actinides

LANSCE should be used to determine the phonon spectra of the various phases of plutonium and other actinides as crystals

become available. These measurements should be carried out over a broad range of temperatures and pressures. This is a long-range goal.

- Crystal chemistry of the actinides

The complex structures of actinide phases should be placed on a more rational basis. LANSCE should be used to determine the crystal structures of plutonium alloy phases that are not yet solved in order to provide fundamental data for this effort.

- Radiation damage in materials

LANSCE should be used to characterize radiation damage in actinides and other materials.

- Texture of materials

LANSCE should be used to measure crystallographic textures of materials that require bulk characterization.

Pulsed Neutron Measurements of Excitations in a Quasi-1-D Antiferromagnet

S. E. Nagler, University of Florida

The one dimensional Heisenberg antiferromagnet is a prototypical example of a quantum many body system. The elementary excitations from the singlet ground state are extremely interesting. The natural excitations are "spinons," with a total spin $S = 1/2$. The spinons are created or destroyed in pairs, with a pair of spinons corresponding to a magnon in the usual description of spin excitations. In systems with integer values of the interacting spins, the spinons are bound, leading to an energy gap (Haldane Gap) in the magnon spectrum, and a dynamical correlation function dominated by a single mode. If the interacting spins are half-odd-integer, the spectrum is gapless, and the dynamical correlation function is considerably more complicated, with a continuum of energies corresponding to each value of wave vector. A real example of the latter system is the insulating salt KCuF_3 , which has $S = 1/2$.

The details of the continuum spectrum in KCuF_3 have been investigated utilizing the MARI chopper spectrometer at the ISIS pulsed neutron source. The quasi-one-dimensional nature of the magnetism is characterized by equivalent sheets of scattering in reciprocal space. If the chain axis is aligned parallel to the incident neutron direction many detectors correspond to points on the same sheet of scattering and can be summed with essentially no loss of information. The time-of-flight method is therefore particularly well suited to the study of low-dimensional problems. The application of this method to KCuF_3 has provided detailed information on the dynamical correlation functions of the underlying model system and supports the theoretical picture of free spinon excitations. Further details may be found in *Phys. Rev. B* **44** (1991) and *PRL* **70**, 4003 (1993).

Glasses and Crystals in Shocked Tuff, Quartz, and Metals

W. J. Nellis, Lawrence Livermore National Laboratory

Underground nuclear explosions at NTS were done in tuft a multiphase, SiO_2 -rich water-saturated rock. Treaty Verification issues, weapons effects in rocks, and the containment of underground nuclear explosions would be better understood and, perhaps, controlled if the structure of the rock surrounding an explosion were known as a function of shock pressure diverging from the source of the explosion. Thus, it is important to determine the glass and/or crystal structure of tuff shocked to pressures up to the Mbar range. Because about 80% of tuff is Si and O_2 in the form of silicates, pure SiO_2 quartz is an ideal simulant of tuff. Tuff and quartz can be shocked with a gas gun at Lawrence Livermore National Laboratory (LLNL) up to Mbar pressures and recovered for characterization of crystal structure and defects at LANSCE. Shock-wave temporal profiles in tuff measured at LLNL have been interpreted in different ways by two different groups (D. Erskine et al., *J. Geophys. Res.* **99**, 15529 (1994)). Both interpretations are obtained by matching different computer models to the same experimental data. One interpretation is that complex buff undergoes a shock-induced phase transition. The other interpretation is that tuff which initially has no strength, becomes an extremely strong material at high shock pressures, without phase

transforming. A phase transition is expected to be irreversible and present after shock. Characterizing this material on recovery from high shock pressure is the only way to resolve this discrepancy. Because of the many phases in shocked tuff and quartz, the high intensity neutron beam at LANSCE is needed. Also, neutrons are sensitive to H_2O and SiO_2 . Basically, the purpose is to understand "knob twisting," the process of making a computer code agree with experiment without providing a physical basis for the agreement.

Also, shocked quartz is the only material in which two different glasses can be made in the same material at the same time with the same chemical composition. Thus, neutron scattering in shocked quartz might provide insight into the nature of a glass, an important technological material.

Similar information should be obtained for materials whose mechanical constitutive properties are needed for accurate computational simulations of these materials undergoing shock loading driven by high explosives. Examples include uranium, lead, tantalum, and steels. Characterization of shock-induced defects are needed to develop constitutive models from first principles.

Plutonium Vibrational Spectra at High Pressures and Temperatures

W. J. Nellis, Lawrence Livermore National Laboratory

Pu and U have numerous phases at high pressures and temperatures, which were identified about 35 years ago with x-ray diffraction up to about 10 GPa (100) kbar. Phonon (lattice-vibrational) data in the solid are needed to try to understand the complex phase diagram of Pu, the most complex of all the elements. Phonon spectra in the solid and structure-factor data in the liquid are needed to improve the accuracy of the interaction potentials between the actinide atoms, which, in turn, are needed to calculate more accurate thermal equations of state. Phonon spectra and structure factors are measured with inelastic and elastic neutron scattering, respectively. Little neutron scattering data exists for the actinides at ambient pressure and no phonon spectra have been measured for the actinides, nor for any other material to my knowledge, at high pressure. Such data are needed in order to determine the variation in a given phase and the effects of different phases. Such data might provide information on lattice instabilities and provide a scientific understanding of the phase transitions. The liquid and six solid phases in Pu at ambient pressure are reduced by applying pressure to only the alpha, beta, and liquid phases above about 2.5 GPa (25 kbar). The face-centered cubic delta phase of Pu, which is stabilized at ambient pressure with Ga impurities, is also important.

Systematic studies are needed for the actinides Th, U, Np, and Pu to determine the effects of different concentrations of f electrons and of different solid structures. Because no phonon spectra have been measured at high pressures for any material, the technique is more likely to succeed first on a simulant such as Ta, which has cubic symmetry.

For the near future, high-pressure and high-temperature work are probably limited to structural and Debye-Waller factor determinations, which have been done, thus far, as a function of temperature at ambient pressure. Neutrons give different and sometimes better powder diffraction patterns than do x-rays because of different scattering cross sections and, thus, scattering lengths.

The dynamics of phase transitions in the actinides might be determined from fast neutron pulses measuring structural phases (diffraction) as the material goes across a solid-solid phase boundary.

The neutron vibrational data would be used by theorists to test calculations. Debye-Waller-factor data as a function of pressure would be new data in which the pressure or volume variation could be an extremely valuable constraint on our theoretical understanding.

The Role of Hydrogen in Earth Processes

C. T. Prewitt, Carnegie Institution of Washington

The presence of water was essential for the origin of life on Earth and for the volcanic, tectonic, and erosional processes that have shaped Earth's surface and determined much of the character of its deep interior. In order to understand the role of water (hydrogen) in Earth's evolution, it is necessary to know how hydrogen-bearing material was introduced and the ability of mineral phases to retain hydrogen under varying environmental conditions.

Two different approaches to explaining how hydrogen might be stored in Earth's mantle are illustrated by a number of papers published over the past 25 to 30 years, but only recently has there been an attempt to provide objective comparisons between the two or to investigate how hydrogen is incorporated into high pressure/temperature phases. One approach invokes the presence in the mantle of dense hydrous magnesium silicates (DHMS) stable at elevated pressures and temperatures.^{1,2} The other involves nominally anhydrous minerals (NAM) that contain hydrogen as a minor constituent on the ppm level.^{3,4} Experimental studies on DHMS indicate these phases may be stable to pressures and temperatures as high as 16 GPa and 1200°C. This temperature is lower than that indicated by a mantle geotherm at 16 GPa, but may be reasonable for a subducting slab. It is possible that other DHMS could be stable to even higher pressures, but little is known about maximum temperature limits. For NAM, small amounts of hydrogen (up to several hundred ppm) have been detected in olivine, orthopyroxene, clinopyroxene, and garnet recovered from xenoliths in kimberlites, eclogites, and alkali basalts;⁴ it has been demonstrated that synthetic wadsleyite and perovskite can accommodate significant amounts of hydrogen.^{5,6}

Questions about models for hydrogen storage include

1. What determines the stability of a phase containing hydrogen?
2. Can NAM retain hydrogen to higher temperatures and pressures than the DHMS?
3. What is the role of cation/anion vacancies in accommodating hydrogen in NAM?
4. What is the effect of pressure on the O-H bond?
5. Is hydrogen present in the mantle a product of the original accretion process or was it introduced by comets or meteoritic material and recycled into the mantle over geologic time?
6. If a solid phase containing hydrogen breaks down at high pressures and temperatures of the transition zone, what is the product—a melt or a fluid or other solid phases?

In addition to infrared and Raman spectroscopy, the most useful technique for determining how hydrogen is incorporated in mineral structures is neutron diffraction.⁷ Except for recent high-pressure studies on brucite, $\text{Mg}(\text{OH})_2$,⁸ we know little about how the hydrogen bond reacts to changes in temperature and pressure. Furthermore, hydrogen appears to be disordered in many mineral phases and probably changes its state of order as temperature and pressure are varied, thus affecting the stability of the minerals involved. Therefore, the availability of neutron diffraction facilities with the capability for high-pressure/high-temperature experiments is essential if we are to make progress in understanding the role of hydrogen in deep Earth processes.

We need to improve our understanding of how hydrogen is incorporated into both the DHMS and NAM. A combination of structure refinement in which hydrogen positions are determined⁹ plus theoretical calculations¹⁰ can provide enough information to establish the immediate environment around hydrogen, resulting in insight about which are the most stable phases and which of the NAM could contain the most hydrogen.

Another kind of model has been proposed for storage of hydrogen in the core, i.e., in iron hydride.^{11,12} Although many investigators discount the possibility of significant amounts of hydrogen being present in the core, one should not overlook the discovery that iron hydride appears to be stable to very high pressures and that an iron hydride composition can explain the seismic properties of the core rather well.

References

1. A. E. Ringwood, A. Major, *Earth Planet. Sci. Lett.* **2**, 130–133 (1967).
2. C. T. Prewitt, L. W. Finger, in *High Pressure Research: Application to Earth and Planetary Sciences* Y. Syono, M. H. Manghnani, Eds. (Terra Scientific Publishing Co. and American Geophysical Union, Tokyo and Washington, 1992) pp. 269–274.
3. R. F. Martin, G. Donnay, *Am. Mineral.* **57**, 554–570 (1972).
4. D. R. Bell, G. R. Rossman, *Science* **255**, 1391–1397 (1992).
5. P. F. McMillan, M. Akaogi, R. K. Sato, B. Poe, J. Foley, *Am. Mineral.* **76**, 354–360 (1991).
6. C. Meade, J. A. Reffner, E. Ito, *Science* **264**, 1558–1560 (1994).
7. J. R. Smyth, R. J. Swope, *Eos Trans. AGU, Spring Meeting Suppl.*, 231 (1994).
8. J. B. Parise, K. Leinenweber, D. J. Weidner, K. Tan, *Am. Mineral.* **79**, 193–196 (1994).
9. L. W. Finger et al., *Nature* **341**, 140–142 (1989).
10. R. N. Abbott Jr., *Am. Mineral.* **74**, 1300–1306 (1989).
11. Y. Fukai, *Proc. Japan Acad.* **59B**, 158–162 (1983).
12. J. V. Badding, R. J. Hemley, H. K. Mao, *Science* **253**, 421–424 (1991).

Complementarity of Pulsed Neutrons and High-Energy X-Rays

D. L. Price, Argonne National Laboratory

The provision of intense beams of high-energy (50 to 150 keV) x-rays from insertion devices in synchrotrons is bringing x-ray techniques into areas of structural and dynamic investigations that have traditionally been the province of neutron scattering. For certain classes of experiments, x-rays can now compete with respect to wave-vector (Q) range, energy resolution ΔE , and ability to penetrate sample containers and environmental apparatus. Recent examples are the measurement of the structure of vitreous silica with 95-keV x-rays at Hasylab, over a Q range of 0 to 25\AA^{-1} , and the determination of vibrational densities of states in α -iron, stainless steel, and SrFeO_x at the Photon Factory in Tsukuba, using an energy resolution $\Delta E = 6\text{ meV}$ and the 14.4-keV nuclear resonance in ^{57}Fe .

These developments should be perceived, not as a threat to the neutron scattering community, but as an opportunity to use the complementary characteristics of neutrons and x-rays (different dependencies of scattering lengths on A and Z , various nuclear resonances, different dependencies of the scatter-

ing processes on polarization) to gain detailed structural and dynamic information on complex materials. At Argonne, we have applied neutron diffraction in conjunction with anomalous x-ray scattering to two complex problems: (a) the short and intermediate order of alkali-modified germanate glasses and (b) the internal structure and relation to the host structure of semiconductor clusters confined in zeolite. In both cases vital information about the atomic structure has been obtained at the partial structure level.

With a new generation of spallation neutron sources, one can expect novel developments in technique that may match some of those recently made at synchrotron x-ray sources. For example, the anomalous scattering technique now being used routinely with x-rays could also be exploited in neutron scattering. About 20 nuclei have resonances in the neutron energy range (0 to 8 eV) covered by a modern glass and liquid diffractometer.

Neutron Scattering Investigation of Magnetism in Artificial Metallic Superlattices

J. J. Rhyne, University of Missouri Research Reactor Center

A significant fraction of the worldwide magnetism research community is currently involved in the study of phenomena associated with artificial metallic superlattices. This includes the study of Giant Magnetoresistance, Interlayer Exchange Coupling, and Strain and Magnetoelastic Effects on Phase Transitions. Typically the superlattice systems of interest consist of alternating layers of a magnetic element (transition metal or rare earth) and of a non-magnetic spacer layer. The thickness of the bilayers and the number of repeats varies widely among the systems studied by neutrons. The question of a phase-coherent coupling of the spins in the dense magnetic layers across the magnetically "dead" layers has been a particularly intriguing part of these investigations, particularly with rare earth superlattices.

Neutrons have proved to have a major impact on our understanding of many of the magnetic interactions in superlattice systems. The techniques of reflectometry and wide-angle elastic diffraction have each provided unique input to the problems. Superlattice perfection, interface roughness, magnetic moment distributions, etc., have been conveniently probed by neutron reflectivity. Coherence effects, effects of strain, and incommensurate magnetic structures have been intensively studied by wide-angle elastic diffraction.

The second very important category of elastic diffraction presents special application challenges for a pulse neutron source. This is an area I recommend that some additional creative attention be paid by future instrument designers. The challenges are the following:

1. The film and superlattice samples are all high-quality single crystals, but of very small volume that presents special intensity difficulties. Instrumental background must be extremely low and well-defined.
2. Typical thicknesses of interest are from less than 400 Å up to 5,000 Å. For a 1-cm × 1-cm sample area, this presents a volume as small as 0.004 mm³. Extinction is not a problem.
3. Magnetic structures encountered may be incommensurate with the crystal lattice requiring a q-space scan trajectory along a particular crystal axis (e.g., (0001) in hcp).
4. Because of the magnetic form factor, measurements must generally be made using the low-q reflections, and proper corrections must be made for the form factor.
5. For coherence information, well-defined line shapes are essential and must be accurately determined including deconvolution of the instrumental resolution.

It is anticipated that future directions in magnetic materials (as well as in many other materials areas) will continue to focus on thin films and superlattices. Because of the neutron's unique capacity to probe magnetic interactions, it is suggested that efforts be made to optimize any new neutron source and its instruments to address the combined challenges of small single-crystal layered structures and magnetic scattering.

SANS Studies of Magnetic Correlations in Disordered Magnetic Systems

J. J. Rhyne, University of Missouri Research Reactor Center

Intense interest has been generated in the last few years in so-called *nanosstructural* materials in which there is a definable length scale of chemical, magnetic, or some other order generally of angstrom dimension. In magnetic materials, the length scale is often produced by a random exchange or random anisotropy interaction that destroys long-range order and produces short-range random magnetic order. This ordering can be conveniently studied by small-angle neutron scattering (SANS), which if properly interpreted, can lead to a determination of the length scale of the magnetic order and a classification of the spin ordering as static or dynamic (fluctuating).

An example of a random magnetic system is provided by amorphous rare earth compounds, e.g., TbFe_2 for which the randomization of the crystal field interaction by the amorphous chemical structure leads to a breakup of the long-range order that is found in the analogous crystalline compounds. For many such random interaction systems, the SANS intensity as a function of Q is of Gaussian form above the ordering temperature as is characteristic of conventional magnetic fluctuations. However, at T_c the correlation function does not diverge as at a normal second order phase transition, rather it is truncated at a finite value limited by the length scale of the magnetic correlations dictated by the random field interactions (a typical value is of order 100 Å). Below T_c the scattering departs increasingly from the Lorentzian form and assumes a behavior that

fits a Lorentzian plus a Lorentzian squared formalism with identical correlation lengths in both terms. This correlation length is typically slowly varying below T_c and decreases on approach to $T = 0$ reflecting the increasing disruption of the longer range order.

The application of a magnetic field in the scattering plane distorts the circular constant intensity contours into ellipses characteristic of scattering from finite range magnetic clusters. The measured correlation lengths (the scattering remains of the Lorentzian + [Lorentzian]² form) actually decrease on application of a field—an effect accompanied by a marked reduction in the intensity of the scattering. This reflects a sweeping of the largest, most easily magnetized, clusters into a semi-infinite cluster by the applied field that corresponds to a near-zero q -value invisible to the SANS. The residual clusters are of smaller dimension, hence the reduction in the measured correlation range.

The instrumental requirements for studying these types of nanostructured magnetic systems are a relatively wide q -range and good intensity, because the samples are often of micron thickness. The wavelength dispersion and time structure of a pulse source SANS are in principle an advantage. Care must be exercised in applying the wavelength-dependent absorption corrections and in isolating the spurious scattering arising from Bragg peaks (sample holder, etc.).

Structure and Dynamics of Liquids and Amorphous Materials

M.-L. Saboungi, Argonne National Laboratory

Liquids, especially those containing H₂, such as polyelectrolytes or aqueous solutions and high-temperature alloys (metallic, semiconductors, or insulators) are materials whose structure and dynamics can be profitably investigated by neutron techniques.

Neutron diffraction from liquids yields information about the survival of intermediate or short-range order with temperature. We have shown that ordering is present in many liquids, and we expect it to occur in some simple systems such as liquid Pu. Determination of the structures at high temperatures is crucial in studying corrosion and long-term stability of materials. The behavior of liquids under extreme conditions (e.g., high-pressure or/and high-temperature) can also be examined by neutron diffraction. Recent experiments on high-T, high-L liquid alkali metals, Li, Hg have led to a reassessment of many critical data including equation of state.

Dynamics of disordered phases yield crucial information for modeling systems, e.g., intera-

tomic potentials. Inelastic scattering measurements performed on metals and alloys undergoing phase transitions with temperature provide valuable data for understanding dynamic diffusion and transport.

Structural determination of liquids and disordered materials requires dedicated diffractometers covering a high Q range with short-wavelength neutrons and detectors at low-angle $2\theta < 45^\circ$ and a comprehensive data analysis procedure. This has been recognized in many neutron sources by building specialized instruments such as D4B at ILL, SANDALS at ISIS, and GLAD at IPNS. Advanced chopper spectrometers being designed and built at spallation sources (PHAROS at LANSCE, MARI at ISIS) are extremely valuable for studying liquid dynamics. Provision of low-angle detectors to measure a large range of energy transfer at low Q is especially important in systems undergoing phase transition.

Studying Materials Under Extreme Conditions Using Neutrons

J. E. Schirber, Sandia National Laboratories

A time-of-flight (TOF) neutron source such as LANSCE provides a unique capability to study phenomena and materials under extreme conditions; for example: temperature, pressure, or radioactivity. This uniqueness stems from the fact that the effects of the dewars/pressure vessels/radiation container etc. can be almost completely eliminated by appropriate shielding so that only the desired sample is observed.

We have used LANSCE and IPNS to study novel materials such as buckyballs and high-

temperature superconductors at high pressures and low temperatures as well as various solid-solid phase transitions. However, these advantages can be applied to various Defense Programs (DP) component studies bearing on safety and surety and the understanding of new materials of interest for DP applications.

We have recently performed pressure studies on C_{60} using He, Ne, and Ar as pressure media.

Neutron Scattering at High Pressure

R. Von Dreele, Los Alamos National Laboratory

The high neutron flux available at the High Intensity Powder Diffractometer (HIPD) affords the possibility of performing powder diffraction experiments at extreme sample environments such as high pressure. We have available a "V3" Paris-Edinburgh high-pressure cell which is capable of producing pressures in the 10 to 30 GPa range and which easily fits in the sample chamber or HIPD. It is equipped with a built-in 240-ton ram allowing pressure changes in situ on the 100 mm³ sample volume. Some recent studies include an examination of the compressibility mechanism in the high T_c 1223-Hg cuprate superconductor to 9.2 GPa in which we observed a substantial shortening of the "axial" Hg-O distance with pressure but little change in the "apical" Cu-O distance despite the substantial increase in T_c

over this pressure range. A second study demonstrated the formation of hydrogen bonds at increasing pressure to 9.6 GPa in the model water bearing mineral brucite, $Mg(OD)_2$, which accounts for its improved stability at high temperatures and high pressures over that at ambient pressure. We also examined the simple model explosive material, d₃-nitromethane, and found differences in its equation-of-state to 5.5 GPa over that of the protonated material which is accompanied by differences in the degree of methyl group ordering. This sampling of studies demonstrates the utility of this cell for powder diffraction studies at high pressure that can be done at LANSCE.