Title: Neutron Structural Biology

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Submitted to: DOE Office of Scientific and Technical Information (OSTI)
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includes the analysis of design parameters for protein and virus crystallography as well as
Neutron Structural Biology
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Abstract
This is the final report of a one-year, Laboratory Directed Research and Development (LDRD) project at Los Alamos National Laboratory (LANL). We investigated design concepts of neutron scattering capabilities for structural biology at spallation sources. This included the analysis of design parameters for protein crystallography as well as membrane diffraction instruments. These instruments are designed to be general user facilities and will be used by scientists from industry, universities, and other national laboratories.

Background and Research Objectives

The aim of this project was to investigate design concepts and identify fabrication pitfalls of neutron scattering capabilities for structural biology at spallation sources. This includes the analysis of design parameters for protein and virus crystallography as well as membrane diffraction instruments. These instruments are designed to be general user capabilities that can be used by scientists from industry, universities and other national laboratories. Both hardware and software have to be user friendly but still exhibit the flexibility needed for future as yet undefined experiments.

The use of large detectors will be a major component of any new spectrometer. At present the typical neutron detector is about 17 x 17 cm with a resolution of 1.3 mm at full width at half maximum. Detector concepts will be investigated that allow at least a five-fold increase in active area. For a planned crystallographic application, a detector with a radius of 70 cm and a 20 cm height covering an arc of 120 degrees is envisaged. Such a detector will have a nearly 10-fold increased active area as compared to the presently used detectors.

In addition to such new detectors, new stations will use focusing optics to increase flux. Such optical systems will be based on supermirror technology. Further increases in flux can be achieved by employing moderators matched to the energy resolution needed for the type of experiments. The concept of using such focusing devices has already been successfully tested for vertical focusing but has to be developed for toroidal geometry to approach point focusing.

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Importance to LANL's Science and Technology Base and National R&D Needs

The continued development of neutron diffraction and scattering science is a designated LANL thrust area. The development of protein, virus and membrane diffraction capabilities is in direct support of this thrust area. These developments for structural biology will strengthen expertise useful in the development of instruments at the Manuel Lujan, Jr. Neutron Scattering Center (MLNSC) and of similar capabilities at the planned Long Pulse Spallation Source (LPSS) at the Los Alamos Neutron Science Center.

There is a major demand for neutron capabilities for research in structural biology in the US from other national laboratories, universities and industry. There are three neutron scattering instruments for small angle scattering but only one instrument for protein crystallography or membrane diffraction. This station is at Brookhaven National Laboratory (BNL) and is only capable of satisfying a small fraction of the external user demand.

Our completed design of neutron scattering capabilities for structural biology forms the basis for a first neutron instrument that will strengthen the Los Alamos structural biology effort and satisfy the DOE-OBER (Department of Energy-Office of Biological and Environmental Research) goal to bring major diffraction tools to the scientific community. OBER has indicated that it is interested in funding efforts in neutron structural science and supports an external users program.

Scientific Approach and Accomplishments

This one-year task resulted in the completed design of a neutron instrument for application to the structural biology effort at Los Alamos. In addition, this capability will provide a unique resource for a future external users program. The detector has a radius of 70 cm and a 20 cm height covering an arc of 120 degrees. This detector has a nearly 10-fold increased active area as compared to the presently used detectors. In addition to detectors such as the one we have designed, new experimental stations will use focusing optics to increase flux. The optical systems will be based on supermirror technology. Further increases in flux are being studied by employing coupled moderators matched to the energy resolution required.