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## Present Status and Plans for Upgrading the Lujan Neutron Scattering Center

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ABSTRACT

The Lujan Center, part of the LANSCE accelerator complex at Los Alamos National Laboratory, operates a comprehensive neutron scattering facility for the U.S. Department of Energy that serves approximately 300 users per year. This paper will discuss the current instruments and status of the facility and also focus on the plans for a major upgrade of the Center including new instruments and enhancements to specific existing instruments. The instrument suite currently includes two reflectometers (one with full polarization), an engineering diffraction machine, a diffractometer specialized to pair-distribution analysis, 2 general purpose powder diffractometers, and 2 inelastic spectrometers. To complement these spectrometers, a full range of pressure, temperature, and magnetic field sample environments is available for users. As part of the planning for a forthcoming enhancement of Lujan Center, a series of workshops have been held over the past year to encourage user input to the design for new instruments as well as major upgrades of existing machines. Many of the planned facilities are designed to take advantage of the Lujan Center 20 Hz pulse repetition rate and cold source moderators, both of which are beneficial for high-resolution instruments using long neutron wavelengths.

### 1. Introduction

The Lujan Center is a comprehensive neutron scattering center operated by Los Alamos National Laboratory for the U.S. Department of Energy – Basic Energy Sciences as a national user facility. In a typical 6 months run cycle it serves approximately 300 distinct users from around the world. Users receive time and the collaborative expertise of the scientific staff based on a proposal review system. The Lujan Center operates with a proton beam current of 100-125 microamperes on a tungsen target, and currently enjoys a greater than 80% reliability. It is part of the Los Alamos Neutron Science Center (LANSCE) that comprises five facilities that make use of the 800 MeV proton accelerator.

The Lujan Center began operations in the 1970s with 7 instruments including probably the oldest presently operating pulse source instrument, the Filter Difference Spectrometer. The Center experienced a major enhancement in the early part of this decade with the development of 7 new or completely rebuilt instruments 6 of which occupied a new experimental room completed in the late 1980s. Today the Lujan Center operates 11 neutron scattering instruments and has 3 nuclear physics beam lines. Four beam lines are available for future development. The present scattering instrument complement as shown in Fig. 1 consists of the following instruments housed in two experimental rooms (ER-1 and ER-2):

A. *Four powder diffraction instruments* -- the Pair Distribution Function Diffractometer (NPDF – FP1), the Spectrometer for Materials Research at Temperature and Stress (SMARTS – FP2), the High-Intensity Powder Diffractometer (HIPD – FP3), and the High-Pressure-Preferred Orientation diffractometer (HIPPO)
B. *Two single crystal diffractometers* -- the Protein Crystallographic Station (PCS - FP15), and the Single Crystal Diffractometer (SCD – FP6)
C. *Two reflectometers* -- the Surface Profile Analysis Reflectometer (SPEAR – FP9) and the full polarized beam reflectometer (Asterix – FP11)
D. *A small angle scattering instrument* [Low-Q Diffractometer (QD – FP10)]
E. *Two inelastic spectrometers* – (Pharos – FP15) and the Filter Difference Spectrometer – FDS (FP7). A third high resolution inelastic chopper machine, the Correlated Phenomena Spectrometer (CPS – FP13) is in a prototype stage.

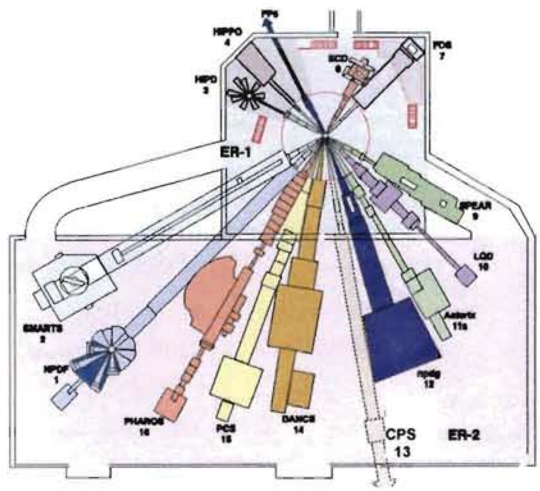


Fig.1 – Lujan Center Instrument Layout in Experimental Rooms 1 and 2

These instruments view five moderators (3 room temperature coupled or decoupled moderators and 2 hydrogen moderators, 1 coupled and 1 partially coupled). A complete new target assembly is currently being installed [2] that is fabricated of tantalum-clad tungsten. It features a new design for the lower tier hydrogen moderator shown in Fig. 2 that includes a water pre-moderator and a cold Be reflector/filter that is calculated to increase flux on the associagted flight paths by 2x.

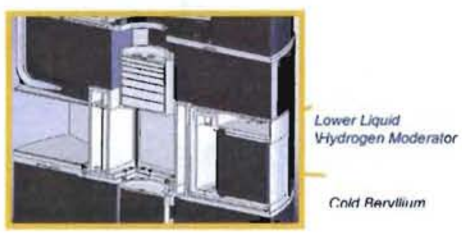


Fig 2. Schematic design of the new lower tier hydrogen cold source part of the new Lujan target moderator assembly.

For the Lujan user program, a strong emphasis has been placed on specialized sample environments that have included have included high pressure capabilities up to 30 GPa from a diamond anvil press, an 11T superconducting magnet that transmits a full polarized beam, and a new 20 mK cryogen-free dilution refrigerator. A Langmuir trough and sheer cells are available for soft matter studies as well as a variety of conventional low temperature cryostats and closed cycle refrigerators and liquid pressure cells.

## 2. Plans for the Future

The Department of Energy – Basic Energy Sciences has designated the Lujan Center to be a second major neutron scattering facility for the U.S. alongside the flagship Spallation Neutron Source. As such it has endorsed [1] a significant enhancement of the Lujan Center instrument complement and associated scientific and technical staff. This goal of this upgrade is to develop up to 3 new instruments and provide major upgrades to an additional 4 bringing the Lujan Center to a planned >90% utilization. As part of the planning for this program, a series of workshops have been held over the past several years to encourage user input to the design for the new instruments as well as for the desired upgrades of existing machines. Many of the planned facilities are designed to take advantage of the Lujan Center's 20 Hz pulse repetition rate and cold source moderators, both of which are beneficial for high-resolution instruments using long neutron wavelengths. Over the past year workshops have been held on the development of (a) a Correlated Phenomena Spectrometer for magnetism and other condensed matter studies, (b) a second pair distribution function diffractometer for local structure analysis (upgrade of HIPD), (c) a radioactive materials diffractometer, (d) neutron spin encoding on Asterix for small Q studies, (e) new directions in small angle scattering instruments, (f) a high pressure diffraction and imaging facility, and (g) a quasi-elastic spectrometer (redeployment of the IPNS QENS machine.) The objective of these workshops is to form instrument advisory teams of interested scientists leading to the development of a "white paper" preparatory to a full proposal for funding

Fig. 3 SMARTS load frame that is capable of applying forces up to 250 kN to massive samples up to 1500 kg. A companion furnace/cryogenic capability provides temperature environments from liquid $N_2$ to 1700 C.

One of the outcomes of these workshops has been a focus on *discipline-oriented* facilities, building on the strong success of SMARTS, which caters principally to the engineering community with its 250 kN load frame (see Fig. 3) with temperature capabilities from liquid $N_2$ up to 1700 C and large sample sizes up to 1,500 kg. An example of a new instrument targeted to the condensed matter/magnetism community is the planned Correlated Phenomena Spectrometer, which is a high resolution single-crystal inelastic chopper spectrometer on a cold source with a full complement of dedicated sample environments. This is to include hydrostatic pressures up to 1.4 Gpa (and/or anvil cells > 3 GPa), temperatures down to 50 mK, and magnetic fields initially up to 15 T (vertical field split pair superconducting magnet) with a future upgrade to the 25-30 T range (a superconductor-resistive hybrid design or all superconducting if the technology becomes available.) All these sample environments would be available simultaneously for extreme environment studies of magnetic or superconducting systems.

A second example of a specialized instrument is found in the highly successful local structure studies performed on the Neutron Pair Distribution fuction diffractometer (NPDF). This technique using Fourier inversion methods to determine local (non long-range averaged) structure from a diffraction pattern taken over a very wide range of scattering wave-vector (Q) has permitted a number of major research breakthroughs in understanding of the structure of oxide, nano-structures, and other materials. Demand for this instrument has far outstripped capacity resulting in a proposal to build a second facility through modification of the HIPD diffractometer.

The power of the local structure analysis technique is illustrated by studies [3,4] of the temperature dependence of the Jahn-Teller distortion of the Mn-O octahedron in the manganite-class of colossal magnetoresistance materials. As shown in Fig. 4 (left pane) conventional "wide-angle" diffraction studies have indicated that the asymmetric Jahn-Teller distortion of the octahedral collapses rather suddenly above about 720K. These measurements average over atomic neightbors throughout the entire bulk material. In contrast PDF measurements utilizing Fourier transform techniques applied to wide Q-range diffraction data allow one to control the range of averaging (x-axis of the data in the middle pane) over which the structure is determined. As shown in the middle pane, for low averaging ranges (e.g, <8 A) no appreciable temperature dependence is observed and certainly no collapse is seen (right pane) as in the diffraction data. This result proved that

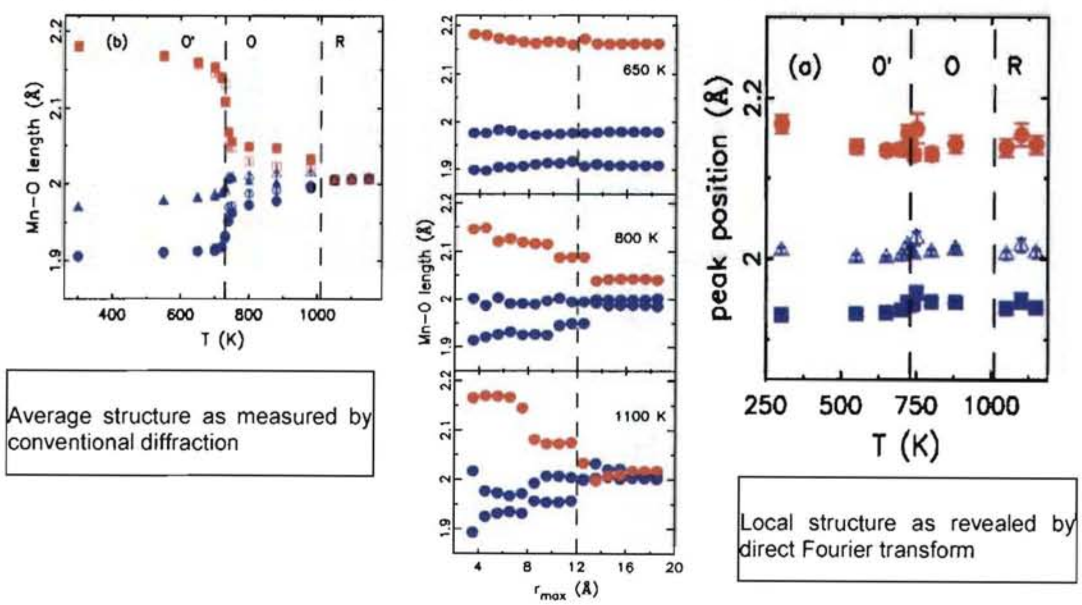


Fig. 4 Local structure determination of the temperature dependence of the Jahn-Teller distortion in CMR manganites. The left pane shows the vanishing of the asymetric distortion in the 800 – 1000 K range as measured by convention diffraction. The right pane showsthe absence of the collapse on the local scale even for T > 1000K. The middle pane shows the dependency of the measured distortion on the range of averaging over nearest neighbors.

it is the thermal averaging of multiple octahedra that produced the apparent collapse of the Jahn-Teller distortion as observed in conventional diffraction data.

The technique of neutron spin-encoding is being developed in collaboration with Indiana University for the Asterix polarized-beam reflectometer. This provides a highly precise measure of small angle scattering from samples and is a real space echnique as opposed to conventional reciprocal space scattering.

The closure of the Argonne Intense Pulsed Neutron Source (IPNS) in 2008 made available several instruments to the Lujan Center. The IPNS single crytals diffractometer has been installed on FP-6, replacing an obsolete single crystal machine, and is fully operational and has provided significantly enhanced single crystal structure determination capability. Components of the POSY-I reflectometer are being incorporated into Asterix including the 3-d vector superconducting magnet assembly that allows magnetizing a sample in an arbitrary direction and also the polarization analyzer. The prototype correlation chopper elastic instrument CHRISTINA from IPNS has been initially tested at FP-12 and is scheduled for additional commissioning runs in the coming run cycle. This spectrometer exploits unique cross-correlation methods of incident beam modulation to separate true quasi-elastic diffuse scattering from other inelastic processes [5]. Another IPNS instrument, the quasi-elastic spectrometer (QENS), is slated for installation on FP-11b; however it will require significant investment in a new guide and shielding structure. User demand for this capability is strong because it is presently unique at US scattering facilities.

**3. The LANSCE-Lujan Center Neutron Scattering School**

The Lujan Center initiated a neutron scattering school in 2004 with a focus on distinct disciplines for which neutron scattering has a major impact. This distinguishes the Lujan school from other schools that have a more general overview of neutron and/or x-ray scattering. The topics addressed thus far have included: Magnetism ( January 2004), Structural Materials (March 2005), Soft Condensed Matter and Structural Biology (May 2006), Hydrogen in Materials (July 2007), Magnetism and nano-materials

Fig. 5 Students and associated staff of the 2009 LANSCE/Lujan Neutron Scattering School.

(July 2008), Phase transitions studied with neutron scattering (July 2009), and Engineering Diffraction (to be held August 2010). The school last for 9 days, and the target audience is graduate students and postdocs (Fig. 5). The school is limited to 30 students and is typically over-subscribed by a factor of 1.5. Funding is provided by the Office of Science, US Department of Energy and the National Science Foundation in collaboration with New Mexico State University. Students listen to lectures each morning by world experts in the particular field. In the afternoon they perform experiments on one of the Lujan Center scattering instruments (see Fig. 6) and analyze the data with the help of the instrument scientist. For the last morning students are divided into experimental groups representing each instrument used, and present a paper on the results of their research. Thesse papers are of exceptionally high quality.

Fig. 6 Students examine the detector system for the HIPPO diffractometer before performing real-time experiments.

## 4. Summary

The Lujan Center is funded by the US Department of Energy Office of Basic Energy Sciences to be a national user facility complementary to the flagship Spallation Neutron Source. Its present instrument complement consists of 11 neutron scattering instruments with 3 beams reseved for nuclear physics research. Seven of the instruments are new within this decade. The Center is currently in the planning stage for a major enhancement of its facilities with an emphasis on (a) strengthening its capability for inelastic scattering particularly for low-E excitations, (b) new or enhanced instruments and associated sample environments catering to a specific discipline, and (c) integrating specific instruments (or components) from IPNS into the Lujan Suite. The overall Enhanced Lujan Project is expected to start in FY09 and be completed in 5-6 years.

## 5. References

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