1 Overview of the BNL NSLS-II

1.1 Introduction and Scientific Overview

1.1.1 Goals and Proposal Precis

This proposal is to construct and then operate a new National Synchrotron Light Source, NSLS-II, at Brookhaven National Laboratory. NSLS-II will be an advanced, highly optimized, third generation, medium energy storage ring with full energy injection for top-off mode operation. NSLS-II will replace the current NSLS facility, which is presently 22 years old and will be 30 years old when we propose NSLS-II to become operational. The X-ray brightness and flux of NSLS-II will be world leading, exceeding that of any other synchrotron light source currently existing or under construction. It will be 10,000 times brighter and have 10 times higher flux than the present NSLS. NSLS-II will meet the nation's need for a high brightness medium energy X-ray source. It will enable structural studies of the smallest crystals in structural biology and provide a wide range of nanometer resolution probes for nanoscience. It will make possible coherent beam scattering studies of the dynamics of condensed matter systems in an otherwise inaccessible regime of low frequencies and short length scales. It will introduce new methods for imaging the structure of disordered materials and of biological systems, and greatly increase the applicability of inelastic X-ray scattering. NSLS-II will be situated in close proximity to the present NSLS building and the new BNL Center for Functional Nanomaterials, forming a research cluster for materials science, condensed matter, biology, and chemistry. NSLS-II will serve the cutting edge science of the nation, and will have a particularly dramatic impact as a vital resource for the strong academic and industrial research community of the Northeast United States.

Section 1 of this proposal presents highlights of the scientific opportunities enabled by NSLS-II. The main focus of this proposal is to describe those scientific opportunities in detail, and that is done in Section 2. Section 1 also provides the institutional and regional context that supports the determination that a new facility is vital to the needs of the scientific community. Sections 3 and 4 describe the new storage ring facility and associated instrumentation required for the cutting edge science in Section 2. Section 5 summarizes the preliminary budget and schedule for the project.

1.1.2 Scientific Opportunities

The unprecedented brightness and flux of NSLS-II in combination with anticipated developments in optics, detectors, and computing power will lead to many advanced experimental capabilities that are not possible today. Access to these new capabilities and the unique infrastructure envisioned for this new facility will have profound impact on a wide range of scientific disciplines and initiatives and lead to many exciting discoveries in the coming decades. Section 2 outlines the grand challenges in these scientific disciplines and the impact that NSLS-II will have upon them. Here we present just a few examples, selected from the hundreds of outstanding challenges described in Section 2, which illustrate the breadth, excitement, and importance of the advances that NSLS-II will lead to.

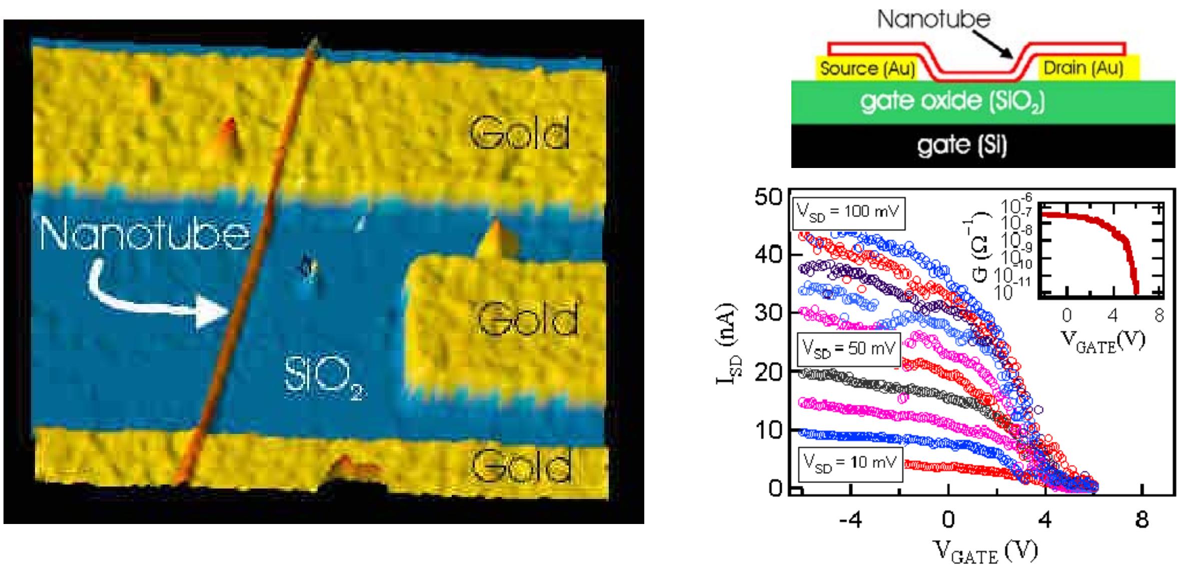

Figure 1.1.1. *(a) Left: Micrograph of carbon nanotube-based field effect transistor (FET). (b) Top right: Schematic of carbon nanotube FET. (c) Bottom right: Demonstration of gate-controlled conductance. The conductance changes by a factor of 100,000 with the application of the gate voltage.*

Nanoscience

The rapid advances in Nanoscience and Nanotechnology promise to revolutionize our ability to control matter on the nanometer length scale and lead to the creation of nanostructures or assemblies that exhibit novel physical, chemical, and biological properties and phenomena. The scientific challenges ahead of us are to understand the unique properties of the individual nanometer-sized building blocks as well as the larger structures and assemblies and to understand the principles of self-assembling so that we can learn to exploit those unique properties and efficiently manufacture and employ the structures.

One exciting example is the possibility of using carbon nanotubes in future electronic and photonic devices. Due to their small size and high aspect ratios (single-walled carbon nanotubes have a diameter of 1.4 nanometer while their length can extend for microns), carbon-based nanotubes are ideal structures to incorporate into FETs and other basic components in advanced nanotechnologies, as shown in Figure 1.1.1(a). However, the electrical and optical properties of the nanotubes are intimately linked with their structure. When the nanotube is stressed, as in the bridging architecture used in the FET depicted in Figure 1.1.1(b), the nanotube electrical characteristics can change considerably. Detailed knowledge of the nanotube structure and electronic configuration will be essential. The unparalleled brightness of NSLS-II combined with recent advances in X-ray focusing optics and new coherent X-ray imaging techniques will enable position-resolved diffraction and spectroscopic investigations of the atomic structure and chemical composition of nanometer-scaled objects such as single-walled carbon nanotube FETs under realistic device operating conditions.

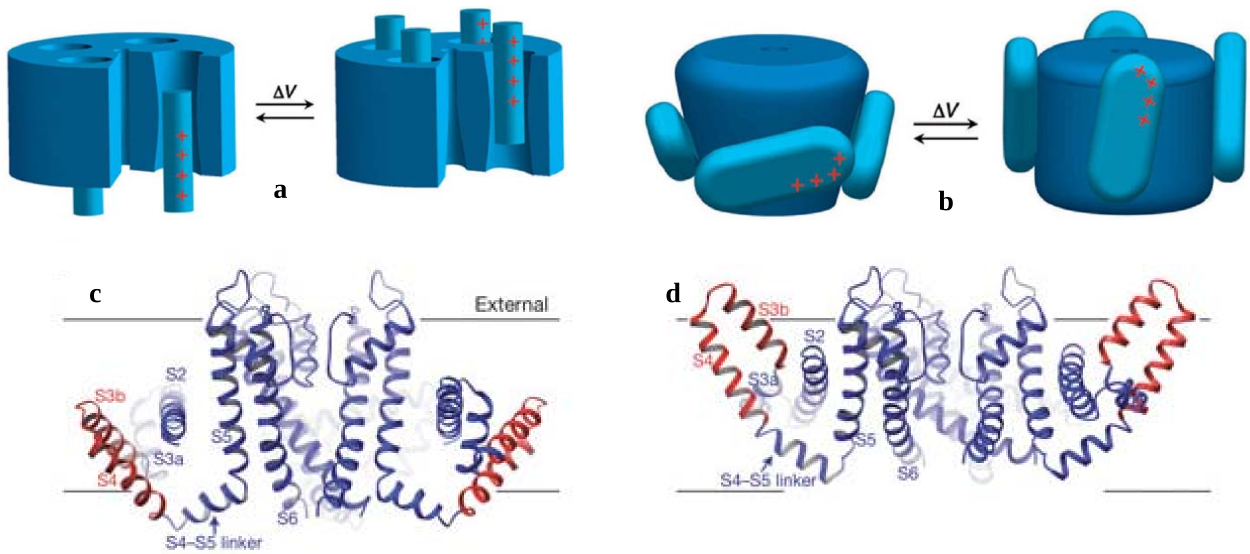

Figure 1.1.2 *Hypothesis for gating charge movements for voltage-dependent K+ channel. a) and b) The conventional and the newly proposed model for gating activation, c) and d) The structure of the channel with the voltage sensor paddles (red) moving across the lipid membrane.*

Structural Biology

Atomic resolution protein structures obtained by macromolecular crystallography are indispensable in advancing many important areas of biological science. The world-leading brightness of NSLS-II will enable researchers to solve increasingly difficult problems.

The work on the voltage-dependent K+ channel (Figure 1.1.2), for which Prof. Roderick MacKinnon, Rockefeller University, was co-awarded the 2003 Nobel Prize in Chemistry, is a perfect illustration of the dramatic impact that X-ray crystallography based structural studies have made in structural biology. Voltage-dependent cation channels open and allow ion conduction in response to changes in cell membrane voltage. Among other processes, these “life’s transistors” control electrical activity in nerve and muscle.

MacKinnon’s work also provides a glimpse into the future, where the most exciting and challenging structural studies will focus on understanding the biological functions of the large number of membrane proteins and large biomolecular assemblies. For example, the largest asymmetric molecular assembly whose atomic structure has been determined to date is that of the whole 70S ribosome, which consists of nearly 100,000 atoms in 53 proteins and 3 chains of ribosomal RNA. Future structural studies will focus on capturing the structure of the ribosome in various functional states in order to fully understand the process of protein synthesis, as well as to determine the structure of the ribosome complexed with antibiotics to facilitate drug design.

With the ultra-high source brightness of NSLS-II, studies such as MacKinnon’s will go beyond static structure to exploration of the dynamics of molecular machines functioning in their natural environments of solutions and membranes, where flexibility of the molecule and water, pH, and ion concentration play determinant roles. Time-resolved studies of macromolecular dynamics and interactions down to microsecond time scales will be possible. These experimental advances, combined with large-scale computer simulations, will provide new insights into the function of molecular machines that carry out critical cellular functions.

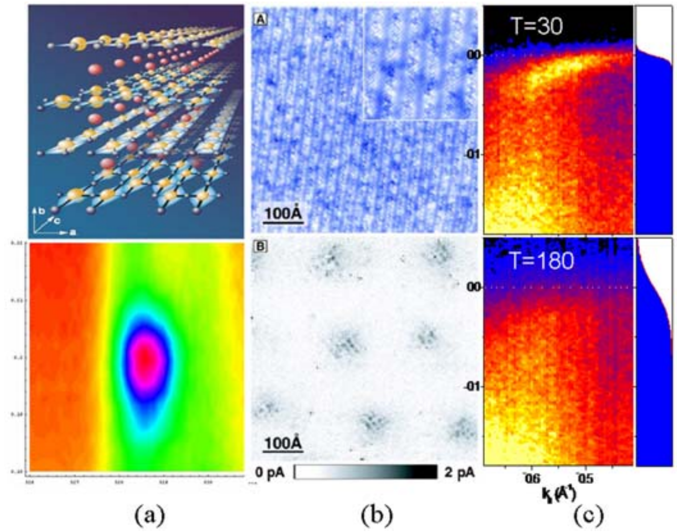

Figure 1.1.3 *(a) (top) 3D model of the spin ladder compound,* $Sr_{14}Cu_{24}O_{41}$ *[1]; (bottom) Direct observation of the proposed charge density wave in* $Sr_{14}Cu_{24}O_{41}$ *using oxygen K-edge resonant scattering. [2]; (b) STM images of vortices in* $Bi_2Sr_2CaCu_2O_{8+\delta}$*, clearly showing modulation with ~2.6 nm wavelength. Soft x-ray resonant scattering at NSLS-II will be able to provide direct evidence of the underlying electronic modulation. (c) ARPES studies of* $Bi_{0.5}Pb_{0.5}Ba_3Co_2O_{9+\delta}$ *show that at low temperatures a two- to three-dimensional crossover in the transport properties occurs [3].*

Strongly Correlated Electron Systems

Understanding the electronic behavior of strongly correlated electron systems is arguably the most challenging problem in condensed matter physics today - one that is driving a revolution in the prevailing paradigm of Fermi-liquid behavior of solids. Since the controlling degrees of freedom in these systems are electronic in nature, probes that couple directly to the electrons are uniquely suited to their study. Further, since these systems are characterized by competing interactions and frequently display inhomogeneous ground states, probes on a number of different length, energy, and time scales are required to fully elucidate their behavior. As a result, the full gamut of synchrotron techniques, including X-ray diffraction, resonant scattering, IR spectroscopy, and high-resolution angle-resolved photoelectron spectroscopy, have provided data which has been critical to understanding these systems.

However, the field is far from mature and surprising new phenomena appear on a regular basis, such as the recent discovery of superconductivity in cobaltate materials, the unusual superconductivity in Sr_2RuO_4, and the realization of “spin liquids”. The transport, thermodynamic, magnetic, and spectroscopic characteristics of these systems are essentially unknown on short length scales and near surfaces. The advances in nanofabrication technology and materials synthesis will for the first time enable researchers to explore low dimensional and finite-size effects in these systems, which might provide the basis for future device applications. For example, one might be able to develop novel sensors and electronic devices based on the metal-insulator, superconductor, and magnetic phase transitions induced by small changes in strain, external fields, and composition.

In coming years, the key to advancing the field will be a strong effort in materials synthesis coupled with the development of new and improved measurement techniques. NSLS-II will significantly enhance the capability of a wide range of experimental techniques, including: ~1 meV high-resolution photoemission using high-energy photons will be possible so that this powerful technique can be applied to a wide range of samples; inelastic X-ray scattering with ~10 meV resolution in the study of electronic excitations will be possible, providing access to an energy scale relevant to, for example, high temperature superconductivity; and it will be possible to use coherent X-rays to study the dynamics as well as image the complex domain structure in these systems.

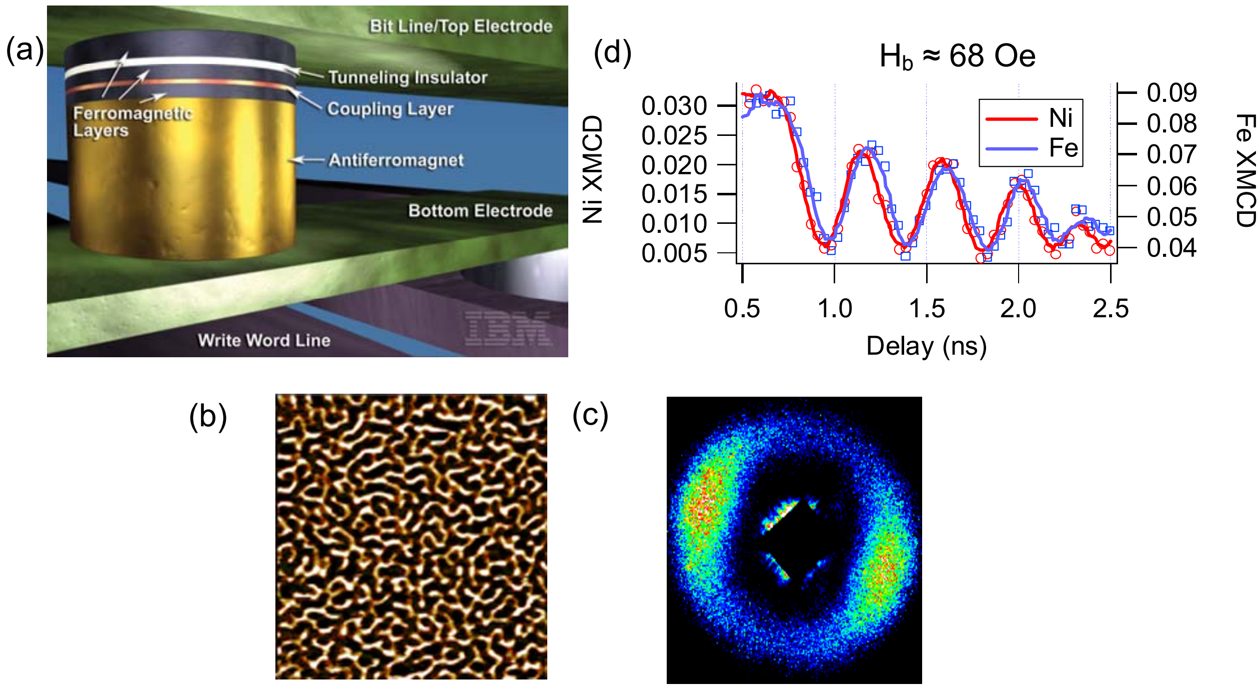

Figure 1.1.4 *(a) Multilayer MRAM structure from IBM. (b) Magnetic Force Microscopy image of the domain structure in a Co/Pt multilayer film. (c) Magnetic speckle pattern from the same sample produced by coherent diffraction of circularly polarized x-rays at the Co L3 edge. The element-specific domain structure can be reconstructed from these diffraction patterns. (d) Element-specific and time-resolved x-ray magnetic circular dichroism measurements of the magnetization rotation for a 50 nm thick permalloy film after application of a fast magnetization pulse. These measurements provide researchers with new insights into magnetization dynamics [4].*

Spintronics

Microelectronic devices which exploit the spin of the electron are still in their infancy in comparison with semiconductor devices. However, they have already had tremendous impact in the area of high-density magnetic storage. Future spintronic devices are under active development and will consist of complex materials, such as the multilayer magnetic random-access memory (MRAM) structure from IBM shown in Figure 1.1.4, spin-polarized field-effect transistors, and fully programmable all-spintronics microprocessors. As element sizes in these advanced magnetic devices approach the nanometer scale and switching speeds surpass the GHz range, designers will be forced to consider fundamental issues such as the magnetic domain structure and the dynamics of magnetization reversal. A thorough understanding of these processes and solution of a number of critical materials issues, such as the development of room temperature magnetic semiconductors, improvements in the spin-injection efficiency across an interface, and understanding spin de-coherence processes, must be achieved before these novel devices can be successfully implemented.

The need to characterize and understand these novel magnetic materials, devices and processes has motivated the development of a wide range of experimental tools using synchrotron radiation over the last decade. The high brightness of NSLS-II in combination with elliptically polarized IDs or polarization conversion optics will significantly improve the sensitivity as well as spatial and timing resolution of these techniques. They will enable study of (1) magnetic interfaces, which play a crucial role in giant magneto-resistance, exchange-bias, and many other important phenomena, (2) nano-scale self-assembled and fabricated magnetic structures, (3) novel magnetic materials, such as molecular magnets, half-metallic materials and magnetic semiconductors, and (4) magnetic switching dynamics.

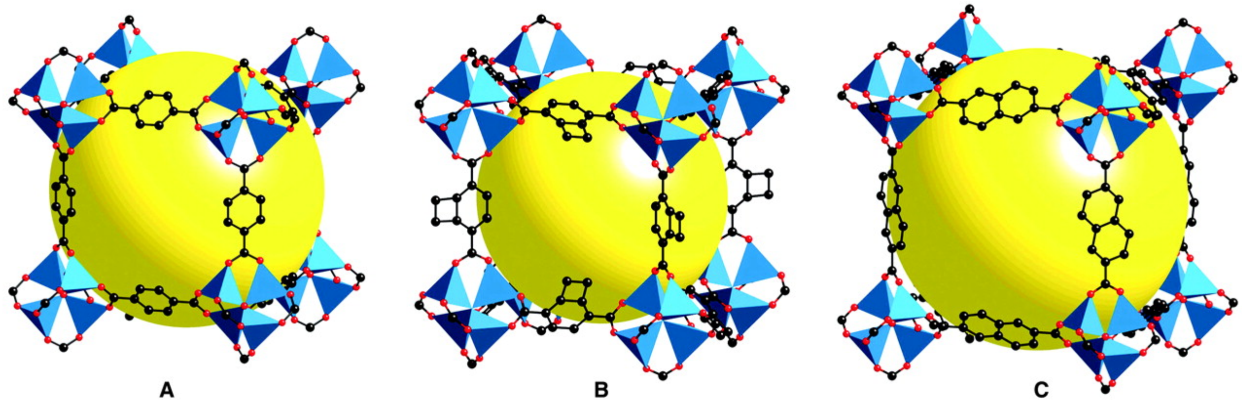

Figure 1.1.5 *An example of a novel metal-organic framework nanostructure used for hydrogen storage. Over 90 % of the crystal volume is open space (yellow ball) which can be used for gas storage (H_2,CH_4,N_2). These are the most porous, and have the highest specific surface area, of any known material. (a) Single-crystal x-ray structures of metal-organic framework-5 (MOF-5) of composition $Zn_4O(BDC)_3$ (BDC = 1,4-benenedicarboxylate) with a cubic three-dimensional extended porous structure which can adsorbed up to 4.5 weigh percent of hydrogen (17.2 hydrogen molecules per formula unit) at 78 k. The topologically similar isoreticular MOF-6 (b) and MOF-8 (c) having cyclobutylbeneze and naphalene linkers, respectively, give approximately double and quadruple the uptake found for MOF-5.*

Energy Research – Hydrogen Storage

In response to the Presidential Hydrogen Fuel Initiative, the Department of Energy's Office of Basic Energy Sciences convened a workshop on hydrogen production, storage, and use in May 2003. The report of that workshop, "Basic Research Needs for the Hydrogen Economy" identified several grand challenges which the scientific community must solve in order to develop and demonstrate viable hydrogen storage technologies for transportation and stationary applications. Among the most important of these are (1) development of novel low-density nanomaterials, which have high hydrogen storage capacity at ambient temperature and low pressure, (2) detailed understanding of the processes by which hydrogen is taken up and released by these complex materials, and (3) development of improved catalytic materials and performance for increased fuel cell efficiency, faster storage kinetics, and increased production capacity. Many promising approaches and materials (Figure 1.1.5) are under intense investigation worldwide, including hydrogen driven metallurgical reactions, chemically bonded complex hydrides, and nanoporous materials such as carbon fibers and nanotubes.

Catalysis and energy science represent perhaps the ultimate challenge for characterization, with reactions occurring at specific atomic sites in a complex system, on short time scales, and at high temperatures and pressures. Nevertheless, it is extremely important to have high-resolution atomic and electronic structures of these materials and their transformation under operating conditions at different stages of the hydrogen uptake/release cycle to aid the search for new materials and understand the adsorption/desorption and reaction/catalytic kinetics.

The unprecedented brightness and flux of NSLS-II will enable measurements with the high spatial, energy, and time resolution necessary to fully characterize these complex systems. Advanced capabilities will include: spectromicroscopy characterization of novel nanocomposite catalytic systems, as well as their active sites and adsorbate-substrate interactions, with better than 10 nm spatial resolution; time-resolved in-situ studies of the kinetics of materials synthesis and catalytic processes on millisecond timescales or faster; application of new experimental techniques, such as high-resolution x-ray emission spectroscopy and x-ray Raman scattering, to provide new spectroscopic information; and the use of combinatorial methods for large scale screening of novel materials.

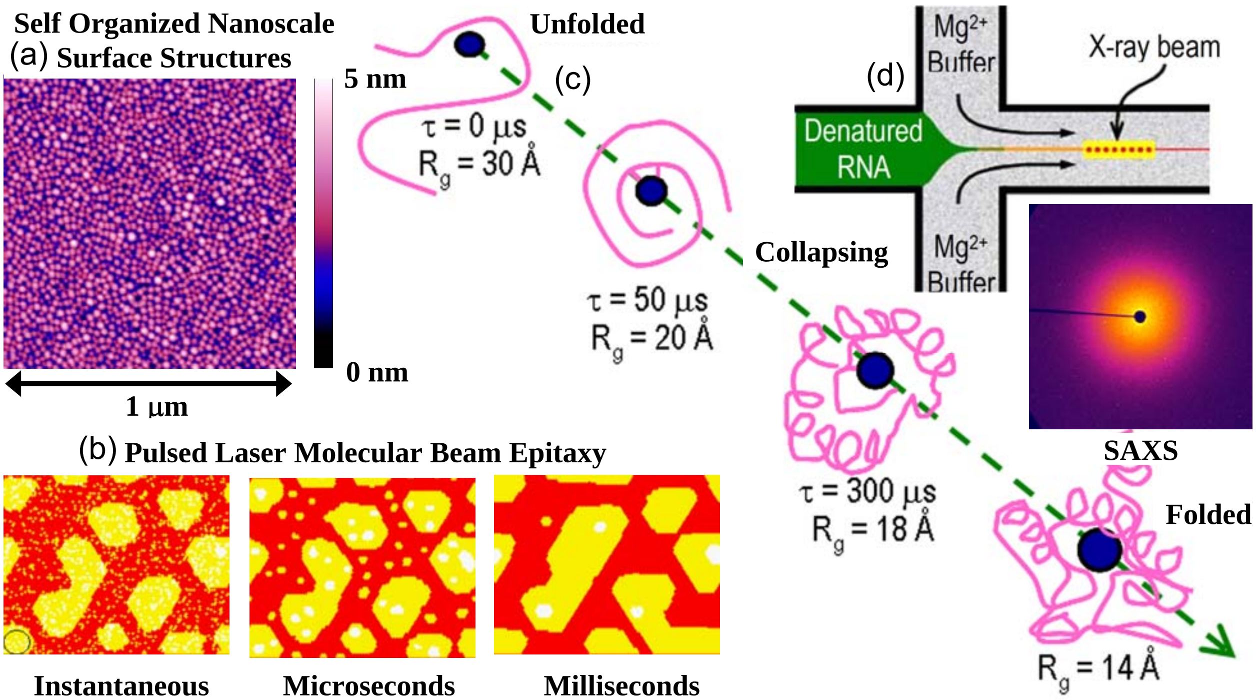

Figure 1.1.6 *NSLS-II will extend studies of many important kinetic processes from the millisecond range possible today down to the microsecond range, providing a region of overlap where computations and experiments can be compared. This will have impact in fields as diverse as growth of advanced materials (a and b above) and understanding of protein folding (c). The high brightness and flux of NSLS-II together with advanced detectors and new experimental techniques such as micro-fabricated flow-cell mixers (d) are key to this advance.*

Kinetics – From Advanced Materials to Protein Folding

Understanding kinetics is the key to unraveling the mysteries of how systems evolve. With current sources, synchrotron experiments are able in many important cases to determine the structural, electronic, chemical, and magnetic evolution of materials with only millisecond time resolution. The high brightness and flux of NSLS-II will extend studies of kinetics into the microsecond regime, providing new insight into a variety of kinetic problems as diverse as protein folding and growth of advanced materials.

For example, understanding how proteins fold is a key to understanding how they perform their biological function. The time scale of the folding process varies from picoseconds to nanoseconds, when the initial secondary structure starts to form, to milliseconds to seconds, when the folding process is complete. Advances to petaflop computational ability will lengthen the time over which folding can be calculated to microseconds. The high brightness of NSLS-II together with advances in micro-fabricated flow-cell mixers will extend the time range over which small angle x-ray scattering measurements can observe folding down from milliseconds, currently, to microseconds. Computations and experiments will then overlap and provide better tests of our understanding of the physics of the underlying interactions.

Similarly, it is crucial to understand materials growth kinetics in order to design materials with ever more advanced properties. In the example of pulsed laser molecular beam epitaxy, deposited atoms diffuse on surfaces on picosecond time scales but surface morphology (islands, terraces, etc) evolves on time scales of microseconds to seconds. NSLS-II together with advanced detectors will allow x-ray scattering techniques to follow the evolution of these nanoscale surface morphologies on microsecond time scales rather than the millisecond time scales possible today. Once again, advanced computations are only able to reach microsecond time scales and so NSLS-II will provide a critical bridge, joining the results of advanced computation with experimental observation.

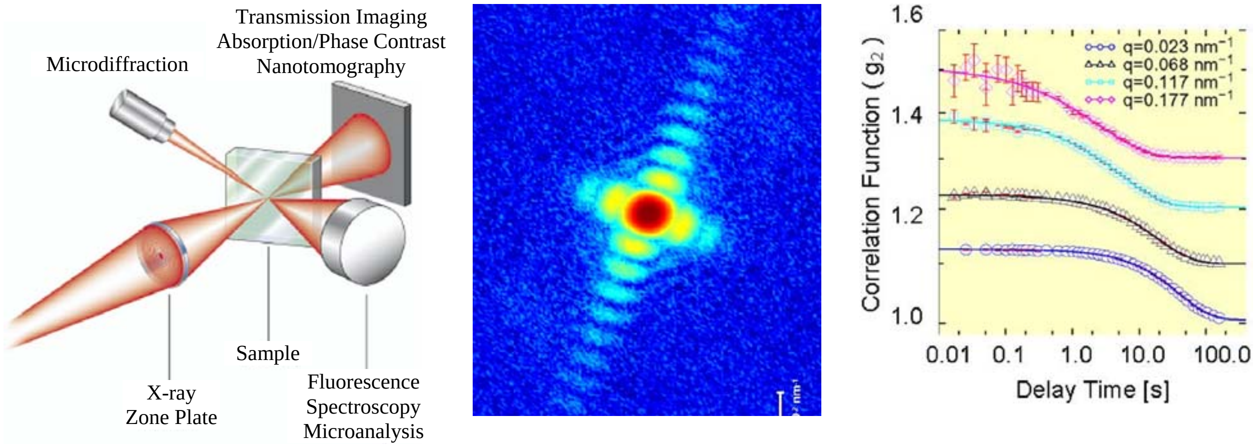

Figure 1.1.7 *(left) NSLS-II will enable nanoprobes to reach 10 nm resolution. (center) Speckle pattern from a 160 nm Ag nanocube. With NSLS-II, coherent diffraction images such as this will provide sufficient information to reconstruct real space images of objects with nanometer spatial resolution. (right) Intensity-intensity autocorrelation functions for an L_3-phase sample of P(SEBS) triblock copolymer in short-chain PS homopolymer. NSLS-II will revolutionize XPCS, pushing the time resolution of studies of the dynamics of soft matter systems from time scales of 10 msec today down to 100 nanoseconds and vastly increasing the diversity of dynamical processes which can be studied.*

Nanoprobes, Diffraction Imaging, and X-ray Photon Correlation Spectroscopy

A hallmark of NSLS-II will be its unprecedented brightness. This singular feature will enable dramatic advances in three particular techniques which find application across all of the scientific areas outlined in Section 2. These are nanoprobes, diffraction imaging, and X-ray photon correlation spectroscopy (XPCS). All require high coherent flux to reach their ultimate potential.

Synchrotron-based X-ray microprobes, with micron and sub-micron spatial resolution, have proven themselves to be extremely valuable research tools. However, by further improving the spatial resolution to 10 nanometers or below, X-ray nanoprobes will, for the first time, allow the characterization of individual nanoparticles or nanometer-sized grains in complex nanomaterials by their density, elemental composition, elemental oxidation state and spin state, strain, texture, magnetization, and atomic and electronic structure and dynamics. This exciting prospect requires the high brightness of NSLS-II to provide a sufficiently high flux of x-rays in the resulting small focal spot.

Diffraction-based (lensless) imaging has the potential to go beyond the resolution of nanoprobes, which are ultimately limited by the laws of optics. With NSLS-II, it will be possible to reconstruct 3D real space images of non-crystalline specimens with a resolution of a few nm. By combining this technique with chemical and magnetic contrast unique to x-rays 3D chemical and magnetic imaging will be possible with similar resolution. Diffraction imaging depends on coherent illumination, and so the high brightness of NSLS-II is essential.

One of the most exciting scientific opportunities offered by the unprecedented brilliance of NSLS-II is its revolutionary impact on our ability to carry out X-ray photon correlation spectroscopy (XPCS) experiments. XPCS experiments at NSLS-II will yield exciting new insights into the dynamics of equilibrium fluctuations of myriad systems, occurring on shorter length scales than can be reached in light scattering and longer time scales than can be reached with the neutron spin echo technique. The ultra-high brightness of NSLS-II together with improvements in experimental technique will revolutionize XPCS, pushing the time resolution from the current state-of-the-art of 10 msec for soft matter systems down to the hundred nanosecond range, vastly increasing the diversity of dynamical processes which can be studied.

1.2 Institutional Context

1.2.1 National Synchrotron Light Source

Designed in the 1970's and commissioned in 1982, the two NSLS storage rings were the first Double Bend Achromat (DBA) lattices and the first second generation storage ring sources in the world. Their design emphasized the production of high flux synchrotron radiation from bending magnets and included only a small number of straight sections for insertion devices. The smaller 800 MeV VUV/IR ring covers the photon energy range from far infrared (IR) to soft X-ray. Continually updated over more than 20 years, the X-ray ring today operates at 2.8 GeV, with brightness several orders of magnitude higher than the initial design value. However, its performance has reached its theoretical limit and its brightness cannot be increased significantly beyond its current value. Additionally, the eight-fold periodicity of the lattice severely limits the number of insertion devices, which are crucial today for producing high brightness radiation.

The NSLS and its successes served as a springboard for 'third-generation' storage ring facilities around the world, many of which scaled up the ground-breaking NSLS lattice. Built with many more cells and insertion devices, these machines today surpass the technical performance of the NSLS.

Today’s most challenging and important problems at the scientific frontier demand photons with a broad spectrum of wavelengths and a broad range of dramatically enhanced capabilities, especially higher average brightness with nearly DC time structure, exquisite position stability, and easy energy tunability for each beamline independent of other beamlines. As described in Section 2, the great majority of the cutting edge scientific problems require photons across the energy spectrum up to ~ 20 keV.

In order to address these compelling scientific challenges, the NSLS proposes development of a new facility that will provide a dramatic upgrade in capabilities relative to the present NSLS. Dubbed NSLS-II, the new facility seeks to preserve the cross-cutting nature of the research that characterizes the present NSLS, while providing the advanced capabilities that are essential to enable the large user community to solve the most challenging scientific problems. This goal can be best realized through the construction of the highly advanced medium energy storage ring proposed here. It will take advantage of the latest advances in storage ring technology, including superconducting undulators, top-off operation, superconducting RF cavities, and others, to achieve world-leading average brightness and flux and set a new performance standard. It will be designed to be upgradeable to operation as an energy recovery linac for even greater performance, should that technology become feasible in the future. Relocating the present VUV/IR storage ring to the new facility to serve as a dedicated IR ring will also provide world-leading high brightness in the important near- to far-IR spectral region. NSLS-II will thus continue to provide one of the unique strengths of the present NSLS, i.e., the broadest range of wavelengths available to users in a single facility, extending from the hard X-rays (0.1 Å), to the far-infrared (10 mm). The wide array of analytical techniques that is currently available to the NSLS users due to this broad spectral range will thus continue in the new facility, with greatly advanced capabilities.

The NSLS scientific and technical staff is highly qualified to carry out this task. The breadth and depth of experience it has gained in operating one of the most successful and heavily used scientific user facilities in the world for the past two decades gives it a keen understanding of the needs of the user community and how to best serve them. With NSLS-II, we will take advantage of the lessons learned at NSLS and other facilities and develop a new paradigm for operating an outstanding user program, including optimization of the respective roles of the facility and users in constructing and operating beamlines. NSLS has routinely operated both storage rings for more than more than 5500 hours/year and with greater than 95% reliability for many years. The NSLS staff has also made pioneering contributions in the pertinent areas of accelerator physics, including development of the first in-vacuum undulators, the first digital feedback systems for beam position stabilization, and many other innovations. The specifications we propose for NSLS-II are ambitious and pose a number of technical challenges. We are confident that we will meet these challenges.

1.2.2 Brookhaven National Laboratory

This proposal builds upon the many strengths of BNL in designing, constructing and operating large accelerator complexes, in developing advanced instrumentation, in carrying out myriad complementary research programs, many of which synergistically interact with and depend upon synchrotron radiation facilities, and in engaging in strong collaborations with the academic community.

BNL has a distinguished history of accomplishments as an accelerator laboratory. Besides the NSLS, other accelerators designed, constructed, and operated at BNL in support of DOE and national missions include the Alternating Gradient Synchrotron (AGS) and the Relativistic Heavy Ion Collider (RHIC), one of the world's largest high energy particle accelerators. Each of these broke new technical ground. All of the expertise, experience, and infrastructure of BNL in executing large scientific construction projects will be available to support the NSLS-II project.

BNL's strength in instrumentation is focused in its Instrumentation and Superconducting Magnet Divisions, which have world class programs in development of new detectors and magnet systems, respectively. The present NSLS has enjoyed a long-standing collaboration with the Instrumentation Division, which has resulted in development of several advanced detectors in use at NSLS today. Even more advanced detectors will be necessary to take full advantage of the high intensity X-ray beams of NSLS-II and continued collaboration with the Instrumentation Division will be central to meeting this challenge. One of the objectives for NSLS-II is to develop and employ superconducting undulators to provide fully tunable radiation from this medium-energy ring. Active development to meet this challenge is underway at the NSLS in collaboration with the Superconducting Magnet Division, Argonne National Laboratory (ANL), Lawrence Berkeley National Laboratory (LBNL), and Stanford Linear Accelerator Laboratory (SLAC).

BNL maintains outstanding research programs in its Physics, Chemistry, Materials Science, Biology, Medical, Energy Science and Technology, and Environmental Sciences Departments as well as hosting exceptional user facilities such as the NSLS, the Center for Functional Nanomaterials (CFN), the Laser Electron Acceleration Facility (LEAF), and others. Many of these research programs either depend directly upon access to the NSLS or interact synergistically with programs that use the NSLS.

For example, BNL's strength in non-synchrotron imaging and other complementary techniques for biological and medical applications, including Positron Emission Tomography (PET), Magnetic Resonance Imaging (MRI), Cryo-Electron Microscopy, Scanning Transmission Electron Microscopy, macromolecular NMR, and mass spectrometry, provide an ideal synergistic environment for structural biological studies and biomedical research that uses synchrotron radiation; several examples are given in Section 2.1-2.3. NSLS-II will stimulate collaboration at every level of biomedical structural study from molecules, to cells, to tissue, to the whole organism, and a vibrant community of researchers will assemble with NSLS-II serving as one of its core facilities.

The Center for Functional Nanomaterials at BNL is a key institutional asset that will benefit NSLS-II both synergistically and directly. The high brightness of NSLS-II is absolutely essential to fully characterize the novel nanomaterials that will be fabricated in the CFN, as described in Section 2.4 and several other parts of Section 2. At the same time, the ability to probe nanomaterials on nanometer length scales will require that the high brightness of NSLS-II be combined with equally advanced X-ray optics to permit the beams to be focused to spots of ~ 10 nm or less. BNL has benefited greatly from a strong collaboration in X-ray optics research, based on advanced electron beam lithography, with Stony Brook University and Bell Labs. The establishment of the CFN will further strengthen this collaboration. In particular, the CFN will house a state-of-the-art electron beam lithography facility that will accelerate the development of a wide range of novel X-ray focusing optics, including zone plates, waveguides, and refractive optics.

1.3 National and Regional Context

In the last decade, there has been tremendous growth in the national synchrotron user community as synchrotron techniques have developed into powerful tools with broad applicability across diverse disciplines. This has been especially dramatic in the Life Sciences, where there has been a large increase in the use of synchrotron radiation in structural biology studies. Structural biology has gained widespread importance, and X-ray crystallography in particular plays a key role in providing physical descriptions of the macromolecular complexes that embody the integrated nature of cellular and functional biology. In coming years, a similar increase in synchrotron usage is likely in the Nanoscience community.

The increasing demand for state-of-the-art synchrotron resources is driven not only by the challenges of highly complex samples, but also by the general growth in the number of researchers who use synchrotron techniques in their research. These trends in growth and usage are shown in Figure 1.3.1 for the collective user population supported by the four DOE synchrotrons: the Advanced Light Source (ALS) and Stanford Synchrotron Radiation Laboratory (SSRL) in California, the Advanced Photon Source (APS) in Illinois, and the National Synchrotron Light Source (NSLS) in New York. Similar trends in growth of users and shifts in usage have been observed at all four facilities. There is every reason to expect this growth to continue and indeed current projections are that the number of synchrotron users nationwide will grow to ~ 11,000 annually in coming years.

At the NSLS, a uniquely diverse and productive scientific community has grown up around it over the last two decades. The wide range of photon energies available at the NSLS brought together researchers from many fields in a comparatively compact environment, fostering collaborations that otherwise might not have come about. Encouraged by BNL and the NSLS, the community blossomed, drawing its strength from the fabric of science and technology throughout the Northeastern US.

Today, the NSLS provides essential scientific tools for about 2400 scientists per year, which is about one third of the total user community for the DOE synchrotrons. These users come from more than 400 academic, industrial, and government institutions. The NSLS user community has gained a well earned reputation for synchrotron based research that is both novel and of high impact. The myriad research

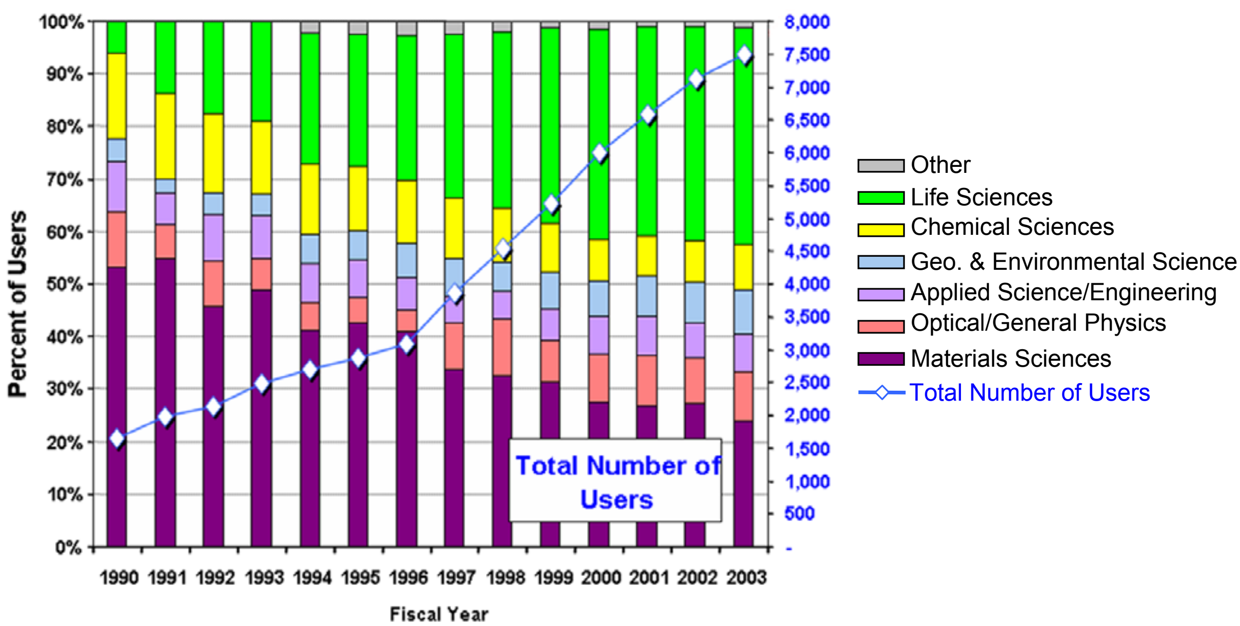

Figure 1.3.1 *User profile by discipline of experiments and total number of users for the four DOE synchrotrons (ALS, APS, NSLS, SSRL). This shows the strong increase in the percentage of users in the life sciences as well as the dramatic growth in total number of users. Current projections are that the total number of users will grow to ~ 11,000 annually in coming years.*

Total Publications	FY2000 824	FY2001 806	FY2002 707
Physical Review Letters	23	18	13
Science	18	12	16
Nature	10	20	18
Cell	11	15	7
EMBO J.	14	20	14
Nature Str. Bio.	15	23	28
Proc. Nat. Acad. Sci.	2	7	18
Structure	5	13	11
Applied Physics Letters	10	10	9
Total Premier Journal Articles	**108**	**138**	**134**

Table 1.3.1 *Research at the NSLS has had high impact. One meaure of that is the number of publications appearing in so-called premier journals. These are listed above with the number of publications appearing in each based on work done at the NSLS for FY2000-FY2002.*

programs of its large user community produce about 800 publications per year, of which about 130 appear in the 'premier' group of international scientific journals, as shown in Table 1.3.1.

In addition to their contribution to the national effort in synchrotron radiation, each of the four DOE facilities also plays a critical role as a vital resource for their region. This is clearly illustrated in Figure 1.3.2, which shows the distribution of users by US State who use each of the four facilities. Almost all users from California use either ALS or SSRL. Almost all users from Illinois use the APS. And almost all users from New York State use the NSLS.

The dominance of the NSLS in the Northeast region is further illustrated in Figure 1.3.3, which shows the geographical distribution of NSLS users. In fact, NSLS is a critical resource not only for New York

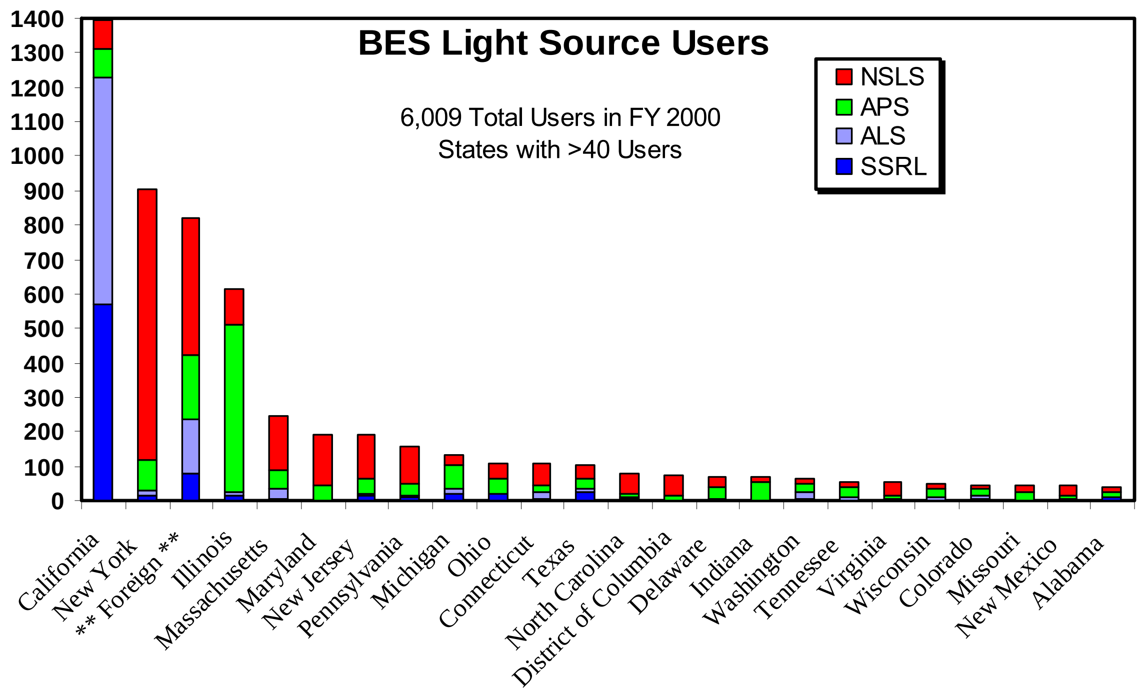

Figure 1.3.2 *Geographical distribution of NSLS users in FY02.*

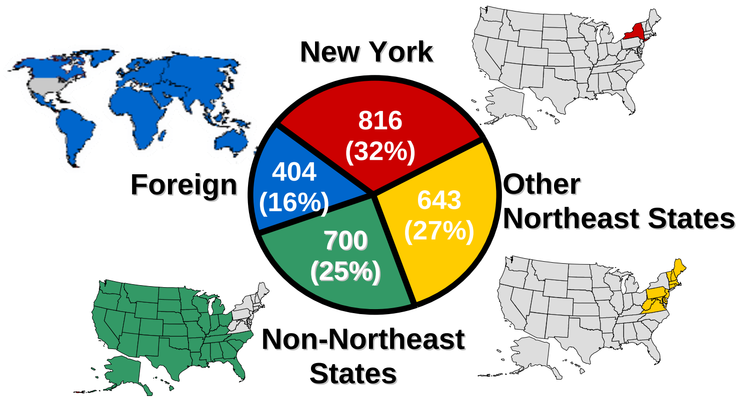

Figure 1.3.3 *Geographical distribution of NSLS users in FY02.*

State, but indeed for the entire Northeastern United States. About 60% of all NSLS users come from Northeast States, with about one third of all users coming from New York State. This illustrates the critical role that NSLS plays as a major resource for this strong research community and as a provider of essential scientific tools to strategic programs at BNL and to neighboring universities. Interestingly, NSLS also draws the largest number of foreign users among the four facilities, representing about 16% of all NSLS users. The remaining 25% of NSLS users come from throughout the rest of the US.

A particularly pointed example of the regional importance of the NSLS is illustrated by the macromolecular crystallography community. As shown in Figure 1.3.4, the NSLS is geographically well positioned to provide resources to a large community of macromolecular crystallographers. One finds that there are about 175 principal investigators from this discipline in these northeastern states, representing 48 universities, 22 companies (mostly pharmaceuticals), and seven other research institutions (hospitals, NIH, etc). As described in a front-page New York Times article on December 30, 2002, the Northeast is "the nation's health care epicenter… stretching from Boston to Bethesda, Md." This regional transformation is reported to have provided the Northeast corridor with a crucial economic cushion during the recent downturn. The Northeast is the site of research facilities for most of the world's major drug

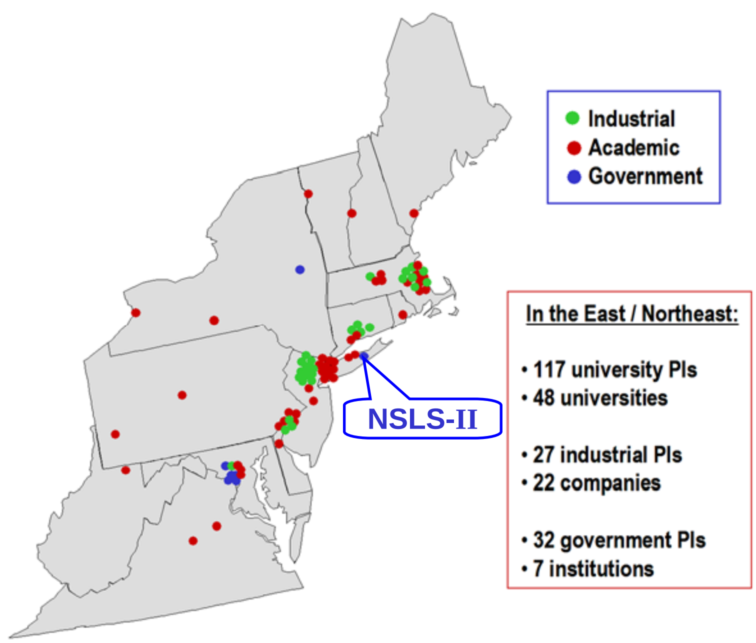

Figure 1.3.4 *Distribution of home institutions of the macromolecular crystallography user community of the NSLS.*

Days of Beam Use	SSRL 2001	CHESS 2001	NSLS 2000	ALS 2001	APS 2001	Row Sums
Canada	3	6	31	0	26	66
Mexico	3	0	0	0	0	3
Midwest	79	0	67	4	366	516
Northeast	39	80	672	5	160	956
Northwest	13	0	124	24	4	165
Southeast	44	2	48	0	33	127
Southwest	34	0	16	1	8	59
West	284	13	32	282	14	625
Totals	**499**	**101**	**990**	**316**	**611**	**2517**

Table 1.3.2 *Synchrotron usage and home institution location, 2000-2001. Taken from the 2002 BioSync Report.*

companies, a very high concentration of academic, government, and private research centers, and biotech companies, most of which are actively engaged in macromolecular crystallography. As part of the Northeastern "health epicenter", NSLS-II will serve as a coalescence site for the biological and biochemical communities in this thriving geographical region.

Data regarding the way investigators tend to employ nearby synchrotron sources is collected in Table 1.3.2. The conclusion is clear: macromolecular crystallographers prefer, and in many cases find it necessary, to collect data close to home. This reduces travel costs and time spent and, importantly, is essential for some cutting-edge projects. The table also shows that in 2000-2001, ~40% of the days used for crystallographic data collection in the US were consumed by groups based in the Northeast. These needs were met largely by NSLS and CHESS, the two increasingly obsolete synchrotrons located in their area. The value of proximate and timely access is very clear to investigators in the region. As was pointed out recently by R. MacKinnon (Rockefeller University), the proximity with the NSLS, and the way this allowed frequent visits to optimize crystal preparation, was absolutely essential for the successful elucidation of the structure of the potassium channel, for which he won the 2003 Nobel Prize in Chemistry. The same sort of iteration argument was made clearly by the Steitz and Moore group (Yale University) a few years earlier concerning their work on the large 50S ribosomal subunit.

The availability of the NSLS to this large research community has dramatically enhanced its productivity. From 1995-2003, there were 4040 X-ray structure depositions to the Protein Data Bank (PDB) from US synchrotrons, of which 1300 came from the NSLS. In 2002 alone, one third of the 880 PDB depositions from US synchrotrons came from research performed at the NSLS. During the last four years, there has been roughly one new structure submitted to the Protein Data Bank *every working day of the yea*r from data measured at an NSLS beam line. Pharmaceuticals express their productivity in a different way: last year seven different companies, mostly from the Northeast, paid for 35 full days of beam time devoted to their proprietary work.

A similar regional need is increasingly being felt in the growing field of Nanoscience. A large number of current NSLS users are engaged in Nanoscience research and this number is expected to increase significantly in the coming decade. As shown in Figure 1.3.5, the Northeast is home to twenty-four major Nanoscience research centers, established by the National Science Foundation, other federal government agencies and various state governments. BNL is poised to be a focal point for much of this research, with the creation of the DOE funded Center for Functional Nanomaterials (CFN) at BNL. With current synchrotron sources, synchrotron radiation techniques are uniquely able to probe the structural, electronic, chemical, and magnetic state of materials on length scales of hundreds of nanometers. NSLS-II will extend the ability of these techniques to probe materials to length scales of 10 nm or less and will be increasingly essential for progress in all aspects of Nanoscience research. In anticipating this demand, several new beamlines and endstations are planned at the present NSLS in close collaboration with the CFN, including small angle X-ray scattering, micro-beam diffraction, and Low Energy Electron and

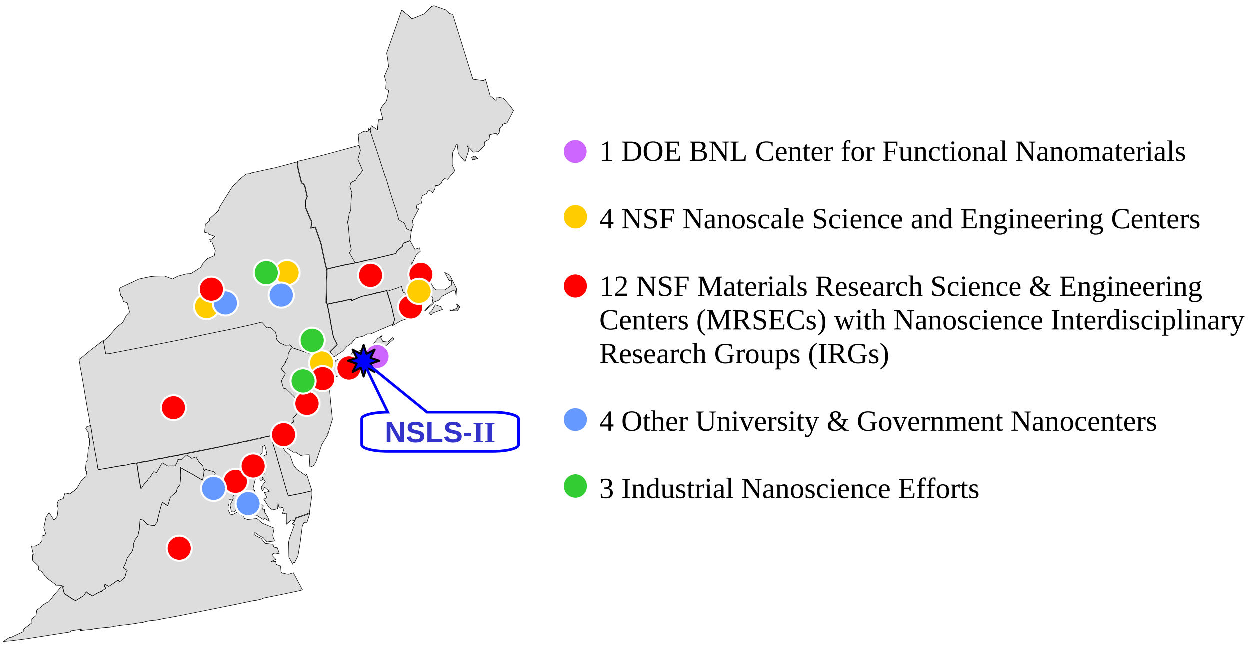

Figure 1.3.5 *Distribution of home institutions of the Nanoscience user community of the NSLS.*

Photoelectron Microscope (LEEM/PEEM). The proximity and strong link between CFN and the NSLS also encourages collaborations among university, government, and industrial researchers.

Demand for synchrotron beamtime is expected to continue to grow across the range of disciplines displayed in Figure 1.3.1. Examples of this are everywhere. The demand for soft X-ray beamtime, particularly for scattering experiments, is expected to grow significantly in the future as resonant techniques are further developed. Advances in coherent scattering and magnetic scattering will also generate larger user communities, particularly in Nanoscience where such techniques will be the only ones capable of probing the electronic behavior with the appropriate resolution. Further, inelastic X-ray scattering techniques to be developed in the coming years will generate communities with the potential to be as active and large as the present angle resolved photoemission community. The soft X-ray undulator at the present NSLS is overwhelmed with proposals unable to satisfy even the existing demand, which even without growth of the community could take the capacity of three dedicated undulators. About 25% of synchrotron experiments in the life-sciences area are non-crystallographic, and this community continues to grow. The techniques that are new and whose value is just being realized, like time-resolved solution scattering, footprinting, and scattering from membranes, will become routine and more widely used as they become more mature. X-ray spectroscopy on transition metals in proteins is an exquisitely sharp tool for dissecting certain information from biological systems, and its popularity will remain strong. The number of user groups that use multiple imaging techniques at the NSLS is a rapidly growing user community, having approximately tripled in the past few years. With the broad spectral range available at the NSLS, the wide range of imaging tools can be combined easily to provide complementary information for sample characterization. This is a feature unique to the NSLS; no other facility in the world has such a wide wavelength range available for imaging. Since synchrotron-based imaging techniques are rather new, this complementarity is just being realized. NSLS-II will continue in this tradition. These are but a small subset of the many examples of increasing demand for not just synchrotron beamtime but also increased capabilities from synchrotron techniques.

Realizing the full potential of these many techniques and scientific collaborations, and enabling even more advanced techniques that are not possible today, requires more than just additional capacity or beamtime. What is critically needed, especially to tackle the most important and challenging problems, is a synchrotron source with greatly increased capabilities.

The capabilities of the present NSLS have been far surpassed by the other three DOE synchrotrons, which are either newer third-generation designs, such as the ALS and the APS, or have been upgraded to third generation capabilities, as at SSRL with its recent SPEAR3 upgrade. The NSLS contribution has continued to be significant in large part because of the sizeable community of Northeast researchers who depend on it. However, the restricted capabilities of the present NSLS are increasingly limiting the productivity and impact of its user community. For the scientific productivity of the large and formidable Northeast research community to continue and even increase, and to tackle the “grand challenge” problems of tomorrow, it is essential that the NSLS be upgraded to provide world leading brightness and higher flux. NSLS-II will accomplish this goal.

1.4 U.S. Scientific Work Force and Participation of Under-represented Minorities and Women

The construction of, and eventually the research performed at, a facility as complex and advanced as NSLS-II will be enhanced by the inclusion of scientists, scientists-in-training, engineers, and technicians from a variety of backgrounds. There will also be substantial training and research opportunities for students and post-doctoral researchers. A healthy exchange of scientific ideas and viewpoints will be fostered by participation of individuals of diverse age, gender, religion, national origin and social backgrounds. NSLS has been the training ground for many of the nations' synchrotron radiation engineers and technicians.

The DOE has a stated mission of providing a workforce of well qualified individuals who meet the specific needs for future scientists and engineers in key technology areas. An integral component of NSLS-II with its advanced technology will be the education of the next generation of U.S.-trained scientists, engineers, and technicians as the Laboratory fulfills this DOE mission. These goals will be accomplished with the assistance of programs administered by the BNL Diversity Office, in concert with similar programs at our collaborating universities.

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