NSLS: first light of its kind!



The year was 1982. Brookhaven National Laboratory (BNL) in Upton, New York was celebrating a milestone at its newest facility: the National Synchrotron Light Source (NSLS) had achieved its first light. It might sound insignificant, like a baby's first sneeze or the first time a pair of newlyweds bought a couch together. But this was a moment that scientists had been building toward for over four years. Batches of electrons rushed through the accelerator

at almost the speed of light. Gigantic magnets bent the path of these electrons into a circle, forcing them to lose energy in the form of x rays. Beam lines directed these x-rays into a detector, towards a brighter future with more science and stuff. Bottles popped, confetti rippled, crowds roared.



Remembering the NSLS, on its last day of operation September 30, 2014, J. Hastings (LCLS, former NSLS R&D group leader, far right) and the "golden boys". The support provided by A. Lenhard, R. Greene, G.

Nintzel, M. Caruso and D. Carlson (absent S. Cheung) through the years to the researcher community has been invaluable.

"It was a whole different world back then," said Richard Greene, a technician who helped to build some of the first beam lines at the NSLS. "We always cracked a bottle of champagne for every beam line."

Before the development of dedicated synchrotron light sources in the '60s, synchrotron radiation was seen as a nuisance in the scientific community. At that time particle accelerators were primarily used to study collisions between certain particles, and synchrotron radiation caused an undesired loss of energy. When scientists realized that they could use this radiation to do different experiments, they began extracting the radiation and using it to study problems in biology, chemistry, material and environment sciences you name it!

"The principle of a synchrotron is that when electrons go around a bend, they lose energy in the form of synchrotron light, which is basically high-powered x rays," said Robert Rainer, who started as a floor coordinator at NSLS and moved on to be one of the lead operators at the NSLS-II. "Those are the x rays that people came here to use at the NSLS, and that they will be using early this summer at NSLS II."

There are three main types of experiments performed at synchrotron light sources: diffraction, microscopy and spectroscopy. Topics ranging from the proteins in your body, to the soil you walk on, to the batteries in your phone and the chips in your computer are being explored at these facilities. A key feature of synchrotron storage rings like the NSLS is a special periodic arrangement of magnets called a Chasman-Green Lattice. Proposed by BNL physicists, Renate Chasman and George Kenneth Green, in the mid '70's, - the Chasman-Green lattice (CG) was fundamental to the development of dedicated synchrotron sources. Designed specifically to enable dedicated synchrotron light sources, the CG lattice is meant to bend and focus an electron beam in the storage ring. Because of its design electrons circulate in this lattice with very low emittance, and the synchrotron light produced is incredibly bright.

"The one thing that always occurs to me immediately with respect to the significance of NSLS at the beginning is the story of Renate Chasman" said Bruce Ravel, a National Institute of Standards and Technology (NIST) physicist. "If we only judged work on its significance, Renate would be completely amazing - the Chasman-Green lattice remained the standard until very recently and NSLS-II in itself is a CG lattice. Of course we live in the real world and in the real world, there just weren't many female accelerator physicists in the late 70s. For me, that puts her in a category that includes mid-century scientists like Rosalind Franklin - a real ground-breaker."

Both Chasman and Green died shortly before their lattice was put to use, for the very first time, in the NSLS. Their work was continued by Samuel Krinsky, who had joined the group in 1976. Sam lead the NSLS accelerator physics group and served on several occasions as interim chair of the Facility. Sadly, Sam, who had been managing the accelerator physics group within the Photon Sciences Directorate since 2008, died shortly before his team achieved a stored current of 50 mA at NSLS II, with a newly installed superconducting radio-frequency cavity in July 2014.

Since its early days it was clear that the NSLS was a game changer. Peter Stefan, a physicist who started working at the facility in 1984 recalls:

"When I first arrived at NSLS, commissioning of the x-ray ring was underway," Stefan said. "We quickly learned something significant about the beam: it carries some real power."

Stefan, who currently works at the SLAC National Accelerator Laboratory, Linac Coherent Light Source (LCLS), explained that many significant technological developments were made at the NSLS in its lifetime. Among these developments, there were small-gap and in-vacuum undulators, which made their appearance in the special X-Ray Ring straight sections. These upgrades, Stefan said, brought about the realization that a missteered electron beam could have the SR beam burn through the storage-ring chamber in milliseconds, and so scientists developed high-speed logarithmic amplifiers on electron beam position monitors so that the orbit could be known over the full range of beam current. They also developed fast radio frequency (RF) trip systems, which enabled a sudden bad orbit to dump the beam before damage could occur.

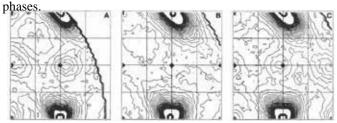
"Such protection systems have been implemented everywhere since then," Stefan said.

Gene Ice (Oak Ridge National Laboratory, ORNL) explained that, "Electron beams of unprecedented low emittance, and consequently much better brilliance than previous sources, together with the outstanding beam stability and specially-built first-oftheir-kind beam lines of the NSLS allowed for crystallography that had previously been possible at only a proof-of-principle level or totally impractical on earlier synchrotron radiation sources." Examples included, anomalous diffraction, surface diffraction, and microbeam diffraction. A great example of early surface diffraction experiments was the studies on X15, which helped pioneer truncation rod scattering.

Ice, a former member of the X14A PRT, one of the very first beam lines on the NSLS experimental floor, remembers that they brought the beamline pre-assembled on rails on the back of a truck.

"We arrived (from Oak Ridge) on a Friday but did not get fully unloaded...The riggers left the forklifts behind, so we finished unloading (the truck) and assembled it (the beam line) over the weekend," Ice said.

Together with X14, the X13 beam lines constituted the first core beam lines dedicated to crystallography. Designed with very revolutionary dynamically-bent sagittal-crystal focusing optics, X14 was specially built for diffuse anomalous diffraction experiments and served to explore a number of new scientific directions such as anomalous powder diffraction, tomographic imaging, quasi crystals, x-ray fluorescence holography...X14 evolved into a workhorse beam line for studies of battery materials, transportation alloys and other materials where anomalous diffraction, high-resolution diffraction and/or highintensity could be used to help identify minor overlapping



One of the first diffuse scattering maps from a single crystals of a nickel-80, iron-20 alloy from X14, the Oak Ridge National Laboratory (ORNL). <u>https://inis.iaea.org/collection/NCLCollectionStore/ Public/19/0</u> 36/19036488.pdf

The X13 beam lines were dedicated to structural crystallography and were later moved to X7 station. X13 A was specifically designed for powder diffraction, and X13 B was dedicated to single-crystal diffraction. The team proposing X13A was a typical PRT formed by members from the University community and BNL (T. Egami, University of Pittsburgh, and C. T. Prewitt, SUNY Stony Brook, and with David Cox, BNL Physics, as



spokesperson). They proposed to the Department of Energy (DOE) a powder diffraction beam line that used energy-dispersive solid-state detectors, along with high resolution, energy-dispersive crystal analyzers and highresolution, angle-dispersive monochromators, to study the structure of disordered materials, phase transformations,

kinetics and structure at high pressure and the crystal structure of inorganic solids. David Cox remembers that the initial proposal was returned without being considered for funding since most of the project was considered of high risk. However, members of the PRT persisted (D. Cox, J. Hastings and W. Thomlinson) performing a series of experiments at CHESS (Cox, Hastings, Thomlinson and Prewitt (NIM, 1983); Hastings, Thomlinson and Cox, J. Appl. Cryst. 1984) to demonstrate the feasibility of the techniques. Subsequently, a high-resolution powder diffraction beam line was commissioned on the X13A port in 1984. This pioneering initiative attracted several companies such as DuPont, Geophysical Lab, CIW, Union Carbide Allied Chemical and later Mobil. The rest is history.



X13B was developed by the BNL Chemistry Department for crystallographic research and started operation in May 1985 with Åcke Kvick (Maxlab Lund, Sweden) as spokesperson. In the early '90's Åcke moved to the European Synchrotron Radiation Facility (ESRF, Grenoble, France). The experimental station included a 6-circle diffractometer and an oscillation camera for data collection on film. The optical components included a double-crystal Si monochromator and Rh coated horizontal focusing mirror. Early protein crystallography experiments with unfocused radiation included the collection of partial oscillation data for the proteins metallothionein, aconitase and ferredoxin in collaboration with Drs. C. D. Stout and A. Robbins (University of Pittsburgh) and W. Dytrych (University of Chicago). In fact the first complete data collection on a protein crystal at the NSLS was performed on the b2 component of the iron containing protein ribonucleotide reductase out to a resolution of 3 A in collaboration with P. Nordlund and his group from of Sweden the Agricultural University (https://inis.iaea.org/collection/NCLCollectionStore/_Public/17/065 /17065212.pdf, p. 228). The group published the structure later in Nature (Nature 345, 593 - 598 (14 June 1990); doi:10.1038/345593a0) to 2.8 Å resolution. However, the first reference in the RCSB to a structure determined at the NSLS was that of the regulatory domain of scallop myosin at 2.8 Å resolution by Cohen's Group on X12C (Nature 368, 306-312 (24)March 1994); PubMed: 8127365; DOI: 10.1038/368306a0; PDB 1SCM). In addition to the protein crystallography experiments, X13 B was used for a broad range of chemical crystallography investigations as well.

The X12 B and C beam lines of the former BNL Biology Department were initially commissioned by Benno Schoenberg (now at Los Alamos National Laboratory), to the NSLS, where J. Hastings (now at SLAC Linac Coherent Light Source, LCLS) and W. Thomlinson (now at Canadian Light Source, CLS) designed and commissioned the optics. R. Sweet built and commissioned the with an Arndt-Wonacott end-station Rotation Camera (Apple-IIc), that he brought from UCLA. For several years the only way to collect data was on film. Always supporting the use of electronic detectors, the X12 Biology Department beam lines, through Sweet, became a natural place for prototype testing or to be one of the first beam lines to own a newly developed detector. The addition of an electronic detector to X12 C and later a cryogenic system to cool the crystals was a real boost to the structural biology program at the NSLS. The small-angle scattering program, on X12 B, was developed by Malcom Capel (now at APS-NECAT), who had joined the biology group in 1985; however by the late '90's the high demand for single-crystal macromolecular crystallography had taken over most of the beam time available on X12 B.

"The X4 beam lines started rather late" recalls Wayne Hendrickson (Columbia University), spokesperson for the Howard Hughes Medical Institute (HHMI) PRT. "The program rose HHMI decided to invest in the work we were doing at Columbia University and I proposed at that time they were talking to me that what we really should do is to build a beam line at a synchrotron to take advantage of the advances that were happening.... The program really took off when Craig Ogata (now at APS) joined us and with a lot of help from Howard Hughes people. Together we celebrated our first successful experiments in 1992."

The X4 beam lines were specially designed for multiple anomalous diffraction (MAD) experiments. X4A was designed to cover a very broad energy range ... "essentially from the Uranium M edge to the Uranium K edge" explained Hendrickson. Using a sagittal focusing monochromator and toroidal mirror this was the beam line for MAD phasing!

Macromolecular Crystallography (MX) exploded at the NSLS in the late '90's. With the advent of reliable cryosystems and better detectors, and further supported by increased funding, the number of PRTs and structural biology beam lines increased to a total of 10 beam lines at the NSLS. Cold Spring Harbor, Los Alamos and NCI partnered with the recently created Protein Crystallography Research Resource (PXRR) to manage several beam lines dedicated to MX. The development of a macromolecular program on insertion-device beam lines by Lonny Berman, Robert Sweet (NSLS II) and the late Paul Sigler (Yale University) on X25 enabled research programs such as those pursued by Mackinnon's group and the groups of Ramakrishnan and Steitz. Anomalous sulfur signal was explored by Z. Dauter (NCI) on the X9 beam line and more recently by Q. Liu on X4. Two new crystallography beam lines were built in the early 2000's: one, X6A on a bending magnet, was built solely by the NSLS with support from the NIGMS, while the second, X29, was built as a partnership between the PXRR, NSLS and Case Western Reserve. This investment contributed to roughly to 1/3 of the user population and approximately 1/3 of the publications.

"Many people, students, post-doctoral and visiting researchers, of various cultural backgrounds, came to the NSLS attracted by the intellectual environment... said Chi-Chang Kao (SLAC).

He himself joined the NSLS as a post-doctoral fellow in 1988 attracted by the vibrant scientific community.

According to Barry Karlin (NIST), who arrived at the NSLS in 1983, "...many graduate students came to be famous scientists..."

Several courses and workshops promoted at the NSLS took on their own identities and were adopted, modified and perfected at other facilities...like the "Rapid Data" workshop initiated by Robert Sweet (NSLS II). Others dedicated to several subjects relevant to special interest groups were organized and highly attended by the community, like the Absorption Spectroscopy workshops organized by Bruce Ravel, Anatoly Frenekel, Simon Bare and Syed Khalid or the Crystallization focus on: ... by Vivian Stojanoff. These courses brought large numbers of graduate students, post-doctoral fellows and scientists together: for many it was their first visit to the NSLS. Smaller workshops like the X6A workbench targeting smaller groups provided a more basic view on MX data collection, along with molecular structure determination, and were further extended to other methods such as with the X9 Small Angle Scattering workshop.

The NSLS had a very dynamic user community and will always have a special place in the memory of those who did their first synchrotron experiments there. The Friday lunch seminars established by Dennis McWhan (NSLS chair 1990-1995; Associate BNL Director 1995-2000) brought the community together. He used to tour the experimental floor on Thursday nights asking users about their experiments and inviting two groups to present their latest results hot of the press! It was a great way to exchange ideas and initiate multidisciplinary research ... but the highlight were the cookies and cakes provided by Carolyn McWhan, Denis wife.

But synchrotron science entered a new era and BNL began phasing out the NSLS in the late 2000's, for a bigger and brighter facility: the NSLS-II. The NSLS-II, which celebrated its own first light in October 2014, is currently considered one of the world's most advanced synchrotrons, producing x rays up to 10,000 times brighter than the NSLS. The new facility is almost half a mile in circumference—nearly five times the circumference of the NSLS. And while the concept of synchrotrons—bunches of electrons propelled by magnets traveling around and around in giant circles—might seem abstract, the consequences of the research done at these sorts of facilities is monumental, affecting everything from technology to human health.

According to Timur Shaftan, an accelerator physicist at NSLS-II, in the early 2000s scientists came to the realization that the NSLS was becoming too old—other machines were providing brighter and more intense x-rays to enable more exciting experiments. So scientists decided to construct a new light source, the NSLS-II, which would support beamlines equipped in a much better way.

"It's a different level of science now," Shaftan said. "Once you have a better source of light you can see much clearer, you can see many more details and have a look at those phenomena that nature hid for us."

Peter Siddons (NSLS-II) has been working at the NSLS since 1985. He was involved in many of the "firsts" devising new

experiments and new detectors. One of the detectors developed by his group, the Maia x ray fluorescence microprobe detector, allows for very fast elemental mapping. High-resolution elemental maps obtained with this detector provided conclusive evidence (*Journal of Physics: Conference Series*, 499, 012001 (2014) (doi:10.1088/1742-6596/499/1/012001) that the painting known as "Old Man with a Beard" was by Rembrandt. Siddons explained that the new synchrotron makes a lot of new things possible. One of these is the spatial resolution... "At the NSLS, scientists could focus the x-ray beam into a 10 micrometer spot. At the NSLS-II, scientists are hoping to focus it down to one nanometer".

"The job of this group is to come up with bigger and better detectors to suit the increased capability of the NSLS-II," he said. This will al-low scientists to study a broader range of samples like minerals, rocks, machinery, biological samples and disease tissues.

The NSLS will always keep its place in history as a landmark in synchrotron radiation. It has been 32 years of successful science and technology. It was a pioneering accelerator that produced world-class science, contributing to two Nobel prizes and had many illustrious visitors, including Rembrandt. It contributed significantly to workforce training and technology development having attracted a number of industries. From whatever angle one may choose to look at the NSLS, its contributions to science, technology and education are undeniable. Historians one day will refer to the NSLS as the accelerator where everything began, shepherded by an enthusiastic team of scientists and engineers who set out to explore new possibilities.



"One thing that really stands out in my mind is the astonishing number of methods that were pioneered in part or completely at NSLS," Ravel said. "Coherent scattering, non-resonant inelastic scattering, infrared spectroscopy, ...Virtually everything we do today at synchrotrons anywhere-including a huge number of things we associate with 3rd generation source-can be traced back to the NSLS."

Alison Sundermier and Vivian Stojanoff

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