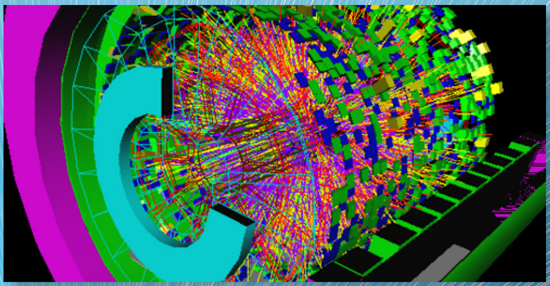
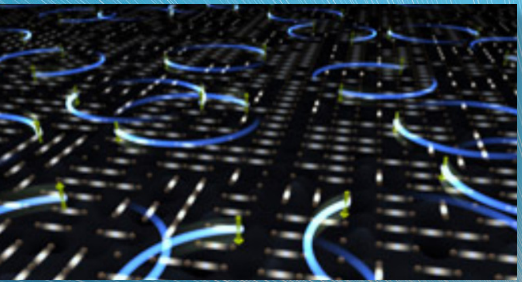
LDRD 2012 Annual Report

Laboratory Directed Research & Development Program Activities

BROOKHAVEN
NATIONAL LABORATORY

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Acknowledgments

The Laboratory Directed Research and Development (LDRD) Program is managed by William Bookless, who serves as the ALD for Policy & Strategic Planning. Preparation of the FY 2012 report was coordinated and edited by William Bookless. He wishes to thank Kathi Barkigia, Patricia Giacalone and Liz Flynn for their assistance in organizing, typing, and proofing the document. A special thank you is also extended to the Production Services Group for their help in publishing. Of course, a very special acknowledgement is extended to all of the authors of the project annual reports and to their assistants.

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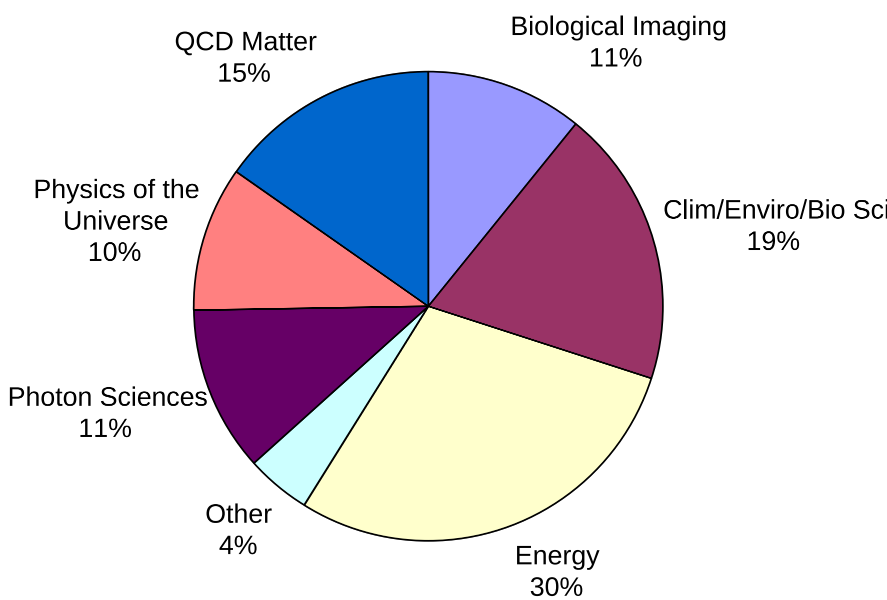
Introduction

Each year, Brookhaven National Laboratory (BNL) is required to provide a program description and overview of its Laboratory Directed Research and Development Program (LDRD) to the Department of Energy in accordance with DOE Order 413.2B dated April 19, 2006. This report provides a detailed look at the scientific and technical activities for each of the LDRD projects funded by BNL in FY2012, as required. In FY2012, the BNL LDRD Program funded 52 projects, 14 of which were new starts, at a total cost of $ 10,061,292.

The investments that BNL makes in its LDRD program largely support the Laboratory's strategic goals as outlined in the BNL Laboratory Plan. BNL has five Laboratory Initiatives; Photon Sciences, QCD Matter, Materials for 21st Century Energy Solutions, Physics of the Universe, and Biological-, Environmental- and Climate Sciences. These major initiatives support the growth and evolution of the major business lines (i.e. mission areas) of the Laboratory. In addition, there are four smaller initiatives that support growth and program development in targeted areas, i.e. Accelerator Science and Technology, Biological Imaging, Computation, and Detectors for National Security. Approximately 85% supported the five major initiatives. In total, these LDRD investments supported 73 postdoctoral researchers and graduates students in whole or in part and resulted in 170 publications and 14 awards.

This Project Activities Report represents the future of BNL science; it is an impressive body of exploratory work that investigates many scientific and technical directions in support of the DOE and BNL Missions. We hope that you enjoy it.



LABORATORY DIRECTED RESEARCH AND DEVELOPMENT

2012 PROJECT SUMMARIES

Nanoscale Electrode Materials for Lithium Batteries

LDRD Project 09-001

Jason Graetz, Yimei Zhu, Xiao-Qing Yang and Weiqiang Han

PURPOSE:

Develop a fundamental understanding of how electrode nanostructure and morphology affect electrochemical performance (e.g. capacity, cycle life, rate capability) and how morphology and nanostructure are affected by lithiation and repeated cycling.

APPROACH:

Our approach is to develop bulk and nanoscale characterization tools to better understand the physical and chemical changes occurring during cycling. Insights gleaned from these studies are used to design new nanostructured electrodes with improved electrochemical properties (e.g., capacity, stability, rate capability, safety).

TECHNICAL PROGRESS AND RESULTS:

Lithium titanate spinel ($Li_4Ti_5O_{12}$; LTO) is a promising alternative anode material for lithium-ion batteries due to its excellent cyclability and safety performance. Its stable framework structure allows reversible lithium intercalation-deintercalation with little change in the lattice parameters. In recent years there has been considerable interest in identifying the location of the lithium and and its migration during discharge, which is often difficult with x-ray techniques due to the low scattering power of lithium. In this study, x-ray diffraction and transmission electron microscopy (Figure 1) were used to measure the local lithium occupancy at different states of charge. During the initial states of discharge (lithiation), the lithium occupying the 8a sites migrates to the 16c sites (above 740 mV). With further lithiation, some lithium re-occupies the 8a sites, initially in the near-surface region at ~600 mV, and then in the bulk at lower voltages (~ 50 mV). The enhanced capacity in nanostructured LTO is attributed to extra lithium storage in the near-surface region, primarily {111} facets.

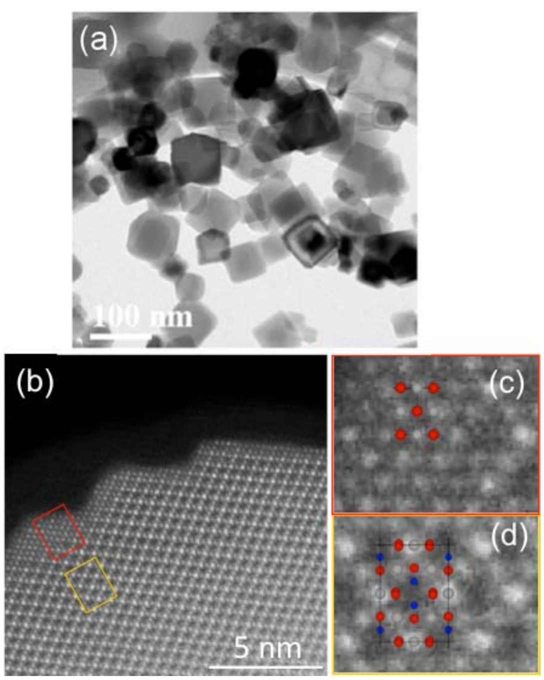


Figure 1. (a) Bright-field TEM image of the pristine LTO nanoparticles; (b) HAADF image from a single nanoparticle, showing the {111} facets. The edge and interior areas marked in (b) are enlarged in (c) and (d), respectively. Although the particle has the spinel structure in the interior (O – red; Li - blue), the structure at the edge (surface) has rock-salt LTO structure. The [110] projection of the spinel and rock-salt LTO structures are embedded in the images.

Photovoltaics: Nanostructure, Solvent Annealing and Performance

LDRD Project 09-003

B. Ocko, C.T. Black, R Grubbs

PURPOSE: Organic photovoltaic devices (OPV) hold great promise as active elements in next-generation solar cells. Two significant factors - both largely structural in origin – limit the efficiency of organic photovoltaic devices, insufficient interfacial surface area between the donor and acceptor and low charge mobility and high recombination rate. Understanding these issues may lead to improved OPV devices with higher efficiency.

APPROACH: Our approach to improving the performance of OPV devices involves (1) developing new materials, (2) providing increased control of the nanoscale phase separation and (3) improving the internal microstructural characteristics of the material. The synthesis effort is led by Barney Grubbs (Center for Functional Nanomaterials (CFN)/Stony Brook University), the electronic device characterization is led by Chuck Black (CFN), and the x-ray scattering effort is led by Ben Ocko (Condensed Matter Physics and Materials Science Department).

TECHNICAL PROGRESS AND RESULTS:

Nano-structured architectures: During the course of this successful LDRD, we have investigated the use of nano-structured architectures to better understand and improve the performance of Bulk Heterojunction (BHJ) OPV devices. The team has had many successes and is considered a leader in the field of how nanostructuring affects OPV material orientation and structure.

X-ray structural studies for PCDTBT thin films, one of the best performing conjugated polymers used in organic solar cells, provide the first report of a bilayer structural motif, composed of a pair of backbones arranged side-to-side where the alkyl tails are on the outer side; a stark contrast to the monolayer ordering found in other conjugated polymers. (published in Nature Communications)

A vertical channel polymer semiconductor field effect transistor architecture was created by confining a conjugated polymer material within gratings of interdigitated trenches where the resulting devices showed near-ideal device operating characteristics with sourcing areal current densities in excess of 40 mA/cm2 using a one-volt supply voltage, a low voltage for such devices. (published in Nano Letters)

Photo-cross-linkable analogues to widely used semiconducting polythiophenes, which were synthesized and shown by X-ray studies and conductivity measurements to be structurally and electronically similar to the parent polymers, were used in bulk heterojunction photovoltaic devices that were found to have improved long-term stability over non-cross-linkable systems. (published in Macromolecules)

The directed assembly poly(3-hexylthiophene):phenyl-C61-butyric acid methyl ester (P3HT:PCBM), materials commonly used in organic photovoltaic devices, investigated on linear grating patterns with domains of alternating high- and low-surface energies showed that the chemical patterns are effective at directing the 3D morphology when the chemical feature sizes are > 200 nm. (published in ACS Nano).

Nanostructured grating surfaces frustrate the molecular orientational ordering within thin films of blended polymer semiconductor poly(3-hexylthiophene) and phenyl-C61-butyric acid methyl ester. Polymer interactions with the surface introduce a 90 degree molecular reorientation at the grating sidewalls, resulting in substrate perpendicular stacking of conjugated pi-orbitals and substrate parallel lamellar packing of alkyl side chains – which we understand through analysis of grazing incidence x-ray scattering measurements. The grating sidewalls strongly inhibit the natural substrate perpendicular lamellar packing of planar films, reducing the relative population of this molecular orientation from 70 percent to less than 5 percent in a 400 nanometer thick film. (in preparation for submission to Advanced Materials).

Nanoimprint lithography (NIL) has proven to be a high-resolution direct patterning technique capable of transferring nanostructures with good fidelity and reproducibility to organic thin films. A re-orientation of the backbone through the use of NIL may lead to improved device performance since it has been shown that the charge carrier mobility is several orders higher in the π-π stacking direction and along backbone chain compared to the lamellar (side chain) stacking direction. In a previous study, we showed that NIL induce a reorientation in poly(3-hexylthiophene) (P3HT) chains. As a continuation of this study, we have now used the same method to imprint blended materials using an inverted device structure. Surprisingly, we show that NIL reorients the polymer backbone in the blend differently than is the case for pure material and that it leads to a sizeable performance increase compared with the planar film. (in preparation for submission to Advanced Materials).

A new small molecule organic semiconductor, 6,6'-bis-(di-(4-methylphenyl)amino)-N,N'-di-(2-ethylhexyl)isoindigo, possesses a low bandgap of 1.57 eV that can be reduced to 1.23 eV by exposure to a small amount of organic acid. The addition of sub-stoichiometric amounts of trifluoroacetic acid to photovoltaic devices prepared from the above molecule leads to an increase in power conversion efficiency from 1.16 to 2.05% (JACS, submitted).

Solar Energy Source Evaluation for Smart Grid Development

LDRD Project 10-006

Meng Yue, Mike Villaran and Robert Bari

PURPOSE:

The purpose of the proposed study is to evaluate the stability, reliability, and power quality of the electrical grid when it is supplied by an increasingly significant contribution from intermittent solar energy generation. The study will also take advantage of a planned BNL solar facility. Systematic approaches featuring probabilistic stability assessment, coordinated control design, and dynamic inclusion of communication infrastructure will be developed. An existing integrated power system analysis tool, EPTOOL, previously developed at BNL, will be expanded and enhanced to facilitate the study of future Smart Grid development.

APPROACH:

The proposed approaches and tasks are discussed for the individual objectives of this study below. The novel features of the proposed approaches include (1) a stability assessment of the grid using of a probabilistic model of a PV system that accounts for its variability; (2) an advanced coordinated wide-area controller design; and (3) an incorporation of communication links into the power system dynamics. In addition, the integrated tool EPTOOL will be expanded and enhanced to facilitate the study of issues related to the Smart Grid development. The plan is to use the BNL solar energy system to provide parameters and data needed for developing and validating models for the PV system. However, hypothetical data can always be used to demonstrate the proposed approach.

TECHNICAL PROGRESS AND RESULTS:

The major achievements of this study in 2012 include

(1) Development of generic dynamics models for solar power generation and battery energy storage systems;

(2) Development of the maximum power point tracking algorithm for solar plants and the grid-tied inverter models and the associated control systems that enable active power injection, reactive power injection including voltage/Var control and power factor regulation. Control schemes for providing other ancillary services such as frequency regulation and/or smooth-out of solar intermittency, low-voltage ride-through etc are also developed;

(3) Development of a simulation-based approach to study the cloud transient induced impacts on the grid responses by assuming that (a) the solar plant consists of a number of arrays (e.g., eight arrays in this study) and all of them are connected to the selected bus; (b) each array is equipped with a power conversion system (PCS) interfacing with the grid; (c) the irradiance level at all panels of a particular array is the same at a given time instant; and (d) the irradiance variation patterns are the same at all arrays but with a time delay at the next array along the cloud movement pathway. The permissible penetration level of solar generation can be investigated using the proposed approach;

(4) Implementation of all of the above models and control systems in a Matlab-based power system simulation software package EPTOOL that performs both power flow and transient stability simulation allowing for a spectrum of grid-integration studies of solar generation and battery energy storage systems.

(5) Development and implementation of more detailed power electronics models as well as solar generation and battery energy storage systems using PSCAD mainly for impact study on distribution network and power quality issues related to solar and battery energy storage system integration.

All of the studies and publications in this LDRD were performed using the EPTOOL and PSCAD. A citing scheme for solar power plants is proposed to minimize the power losses by deploying the plants near the buses that are the receiving ends of the transmission lines with the biggest power losses in the case study using an example system. In this case study, a single solar power plant consisting of eight arrays is connected to bus 37. The penetration level is increased by scaling up the capacity of the solar plant, i.e., increasing the number of solar panels connected in parallel at each array of the solar plant. The transient responses at different solar penetration levels are simulated by applying the same irradiance variation repeatedly to the arrays. The frequency deviations at the POI (Bus 37) are plotted in Fig. 1.

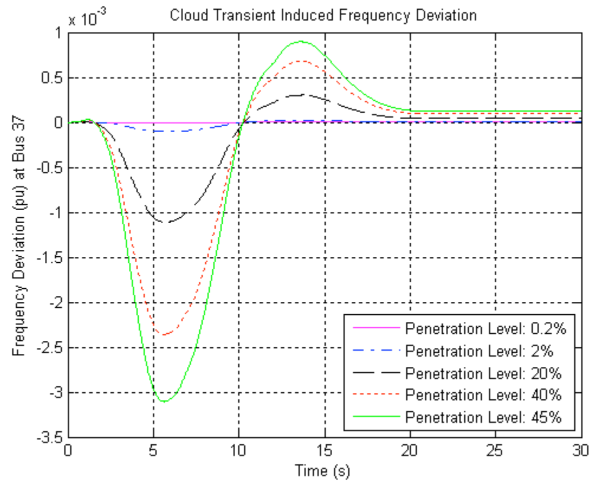


Fig. 1. Frequency deviations for a solar plant at different penetration levels.

Fig. 1 shows that when the penetration level approaches 45%, the frequency deviation caused by the cloud transients alone can be as large as 0.3%, i.e., the lowest frequency (or the frequency nadir) is around 59.8 Hz. This large frequency excursion is not acceptable for some utilities since it increases the risk of under frequency load shedding, cascading outages, or the quick disconnection of the PV plants from the attached grid. Apparently, the frequency nadir may be considered a metric for the grid frequency performance to determine the permissible solar penetration level considering the regional cloud transient patterns for a particular system.
Note that the grid possesses sufficient reserves as none of the generators or the excitation systems reaches its limit. The deep frequency excursion is simply due to slow responses of the conventional generators.

The issue of grid frequency responses to renewables variation including wind has received many concerns. The cloud transient impact may be more severe, i.e., a lower frequency nadir, because of many factors including (1) the irradiance variation may be larger and the subsequent reduction in total solar generation may be much more significant than that in this case; (2) the increase of solar penetration may put some conventional generators offline in light load conditions, which is preferred from the economic perspective, and total inertia is therefore smaller; (3) a disturbance may occur in the same time as the cloud transient does; and/or (4) many generators do not participate in governor responses in practice and/or the system governor response has been declining constantly in some areas of U.S. for many years before the rapid increase in renewable generation. The method and tool developed in this LDRD will enable the study of such grid responses for different penetration levels of solar generation.

High Throughput Quantitative Biochemical Phenotyping

LDRD Project 10-007

Alistair Rogers

PURPOSE:

This LDRD established a platform for high throughput biochemical phenotyping. There are only three labs world-wide using robots to conduct automated biochemical and enzymatic assays, Dr. Rogers' lab is one of them. This LDRD established Brookhaven as the technical leader capable of addressing large scale phenotyping projects. Publications will demonstrate the capability of the platform to address critical questions in global change plant biology focused on central C and N metabolism. The analytical capabilities developed here complement existing analytical assets in plant systems biology at Brookhaven and can be readily adapted to address other challenges in plant biology at the intersection of climate, energy & environment.

This LDRD was completed on September 30th 2012.

APPROACH:

The project had three components (1) Set up a robot that is capable of conducting high throughput biochemical phenotyping, (2) identify and develop assays for diagnostic parameters of interest and adapt them to a 96-well format, and (3) use the platform to address science questions that will demonstrate the utility of the platform. In support of components (1) and (2) Dr. Rogers collaborated with Dr. Gibon (INRA-Bordeaux) who pioneered the use of robots to conduct biochemical assays in plant tissue. In support of component (3) Dr. Rogers collaborated with Dr. Leakey and Dr. Ainsworth (UIUC) on a projects where soybean has been grown at elevated [CO_2] with and without water stress and at high ozone concentration. These two collaborations have resulted in two publications. Dr. Rogers also collaborated with Dr. Zhu (PICB, Shanghai, China) to understand metabolic controls on yield in rice and at Brookhaven Dr. Rogers collaborated with Dr. Schwender (Biology). He is also leveraging sampling conducted as part of his own funded research into carbohydrate profiles in loblolly pines grown at the Duke Forest FACE experiment. .

TECHNICAL PROGRESS AND RESULTS:

Component 1

During the first year Dr. Rogers hired a post-doc, defined the technical specifications of the robot and purchased it. He also began renovation of his laboratory to accommodate the new equipment. This included removal of two old plant growth chambers, repairs to the flooring, and upgrades to the electrical supply and purchase of a second -80°C freezer. In the first quarter of the second year the robot was installed and commissioned. Infrastructure upgrades continued in year 2 and year 3. These included installation of a water supply and drainage lines to the two robots, purchase and installation of cryogenic grinders, purchase and installation of a plate reader cluster.

Component 2

At the onset of the LDRD project Dr. Rogers' lab had 96-well assays for c. 25 parameters of interest in central C & N metabolism. In the first fifteen months of the project his laboratory has expanded this to include nine parameters associated with oxidative stress, five associated with the PEP branch point in central metabolism, four associated with the C4 pathway and three additional parameters associated with N metabolism. Additional parameters continue to be added and existing assays adapted for automation.

Component 3

The assays for oxidative stress were developed in collaboration with a graduate student at UIUC and were used to understand the impact of elevated [CO_2] and chronic ozone exposure to acute oxidative stress. This work has resulted in a paper (Gillespie et al. 2011). Collaboration with Dr. Leakey resulted in a second paper (Gray et al. 2013) and another is in preparation. Analysis from Duke Forest FACE, the rice project (Dr. Zhu) and the *Brassica napus* project (Dr. Schwender) has been completed and manuscripts are in preparation.

New collaborations and funding opportunities

- Dr. Rogers was able to leverage the analytical capabilities developed in this LDRD in a recent award from DOE (Next Generation Ecosystem Experiments-Arctic) \$350,000 y^{-1} (FY12 – 14).
- The LDRD platform enabled Dr. Rogers to form a new collaboration with Dr. Cseke (UA-H) and a preproposal has been submitted to a BER/DOE call.
- The LDRD platform enabled Dr. Rogers to form a new collaboration with Drs. Cumming and DiFazio (UWV) and a preproposal has been submitted to a BER/DOE call.
- A new unfunded collaboration has been started with Dr. Osborne (University of Sheffield, UK) to understand biomass production in C3 and C4 grasses.

Development of an Ultrafast Electron Diffraction Facility for Condensed Matter Physics Challenges

LDRD Project 10-010

J.P. Hill (CMPMSD), X. Wang, J. Murphy, C.-C. Kao (NSLS), Y. Zhu (CMPMSD),
A. Cavalleri (Max Planck – CFEL & U. Hamburg)

PURPOSE:

The goal of this LDRD is to develop a unique Ultrafast Electron Diffraction (UED) instrument to study insulating ground states and fundamental photo-induced excitations in a class of materials called strongly correlated materials. The ground states in these materials are characterized by long range ordering of charges, orbitals, spins and lattice distortions. Using electron diffraction we will probe several of these ordered degrees of freedom in a single diffraction pattern, allowing us to understand how optical radiation couples to these materials and how energy is subsequently distributed. Our instrument is based on a radio frequency (RF) photocathode, providing 100 femtosecond pulses of electrons at 2-5MeV, an order of magnitude higher in energy than all existing UED instruments. At high energies, space charge effects are reduced and shorter pulses can be achieved at large pulse charge. Once operational, this instrument will form the backbone of an ultrafast program within condensed matter physics and material sciences. Based on this work, it is anticipated that a proposal for a new FWP will be submitted to DOE BES to carry out a new program in ultrafast science at BNL.

APPROACH:

The primary objective is to study the novel orderings of charge, orbital, spin and lattice distortions in strongly correlated materials and understand how optical radiation perturbs these ground states and leads to non-equilibrium phenomena. There are no instruments that can accomplish all of these tasks in a simple, compact configuration. Table-top, optical, pump-probe experiments can infer dynamics but can't singly probe a discreet degree of freedom. X-ray methods can probe single degrees of freedom but can do so only one at a time and several ordered degrees of freedom are inaccessible (they lie outside the Ewald sphere). Ultrafast electron diffraction fills this instrumentation void. Using UED, we probe several degrees of freedom independently in a single diffraction pattern, allowing us to understand how the excitation process affects different degrees of freedom on fundamental timescales.

There are several existing UED instruments capable of generating ultrafast pulses of electrons. However, in nearly every instance, these are pulsed sources based on DC acceleration of electrons with maximum achievable energies of 10s of keV to 100keV. While these instruments have contributed important science, there are several shortcomings associated with low kinetic energy electrons. Most importantly, at these energies, pulses of electrons suffer from Coulombic repulsion and hence, the pulse length is strongly dependent on the charge per pulse. Additionally, at low energies the electrons have reduced penetration depth requiring experiments to be performed at grazing incidence in reflection geometry. In recent years, questions have been raised about results obtained from these low energy systems. Specifically, it was proposed that in the grazing incidence geometry, deflection of Bragg peaks (that might imply a deformation of the lattice) could also be caused by a low density plasma near the surface of the material. These unbound electrons near the surface (photo emitted electrons) are exactly what occur when the sample is photo excited.

In collaboration with scientists from the Source Development Lab of the National Synchrotron Light Source, we have constructed a high-energy, short-pulse, electron source based on an RF photocathode. There are several advantages to using a high energy (2-5MeV) electron source. For one, electron pulse length can be finely tuned by varying the phase of the RF driving field relative to the time the electrons are emitted from the photocathode giving us fine control over the pulse length. Additionally, at high energies the increased electron penetration depth allows us to perform these experiments at normal incidence and in transmission, reducing spurious effects caused in the optical excitation process.

TECHNICAL PROGRESS AND RESULTS:

During the first fiscal year (FY10) of this project, we hired a post-doc, Ron Tobey and nearly completed construction of the instrument. We also carried out closely related experiments using optical-pump, Raman probe here at BNL, and optical pump, soft x-ray probe at the LCLS. In FY11, we completed construction of the UED apparatus and observed the first superlattice peaks from a charge density wave system. Since Ron Tobey left to take a faculty position at Groningen University, Netherlands, we hired a visiting post-doc, Pengfei Zhu.

In the past fiscal year (FY12), the signal-to-noise was further improved such that charge and orbital order superlattice peaks were observed in $La_{0.5}Sr_{1.5}MnO_4$ for the first time. This is a dramatic step and means that the system is now ready to carry out real experiments on systems of relevance to condensed matter physics. The first optical pump experiments were then carried out (Figure 1). These demonstrated the overall time resolution of the instrument, including all sources of jitter to be sub 300 fs. Scientifically, the results were also significant showing that the orbital order melts in a non-thermal process following electronic excitation, with a time constant of a few hundred femtoseconds. These results complement similar data taken by us at the LCLS using soft x-rays, with the difference that in the UED experiment we also obtained the behavior of the Bragg peaks to track the lattice behavior. These results are presently being written up for submission to Phys. Rev. Lett. A second paper is also in preparation describing the instrumentation development. The success of this effort has, in part, motivated the development of a white paper to build an ultrafast THz facility at BNL with UED as a flagship endstation at that facility.

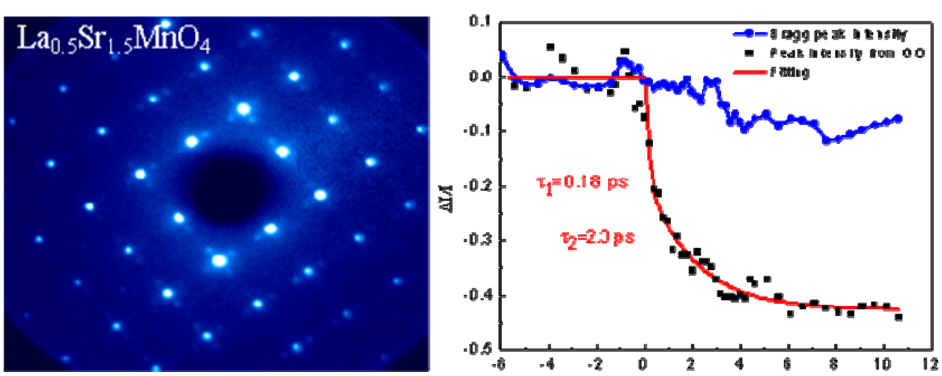


Figure 1: Left panel, diffraction pattern from $La_{0.5}Sr_{1.5}MnO_4$ showing 4-fold orbital order superlattice peaks around each Bragg peak. Right panel Bragg peak (blue) and orbital peak (red) following optical excitation pulse at t=0 ps.

Design of Pt-free Electrocatalysts for Fuel Cell Oxygen Reduction Reactions

LDRD Project 10-012

Peter Khalifah

PURPOSE:

The objective of this work is the synthesis and characterization of a number of novel conductive and acid-stable transition metal oxide systems to explore their potential for electrocatalysis. Although Pt-based hydrogen fuel cells have demonstrated impressive efficiencies (~60%), the current technology can never be implemented on a commercially relevant scale due to the extreme cost and the terrestrial scarcity of the platinum metal that is used to catalyze the recombination of protons with O_2 to form water in the oxygen reduction reaction (ORR). Furthermore, the ORR reaction is inefficient and requires a very large overpotential to proceed. A search for better catalysts is being pursued, integrating the materials synthesis and discovery experience of the Khalifah group with the fuel cell electrochemistry measurement expertise of the Adzic group. This search focuses on conductive transition metal oxide systems which offer the promise of activity, economy, and acid stability necessary to produce viable fuel cell systems. The search for effective new catalysts is a high-risk exploratory project, but one which can potentially offer large rewards. Success in this endeavor will provide the preliminary results necessary to compete for programmatic funding in this area, and will establish a strong collaboration between synthesis (Khalifah) and characterization (Adzic) groups in the BNL Chemistry Department.

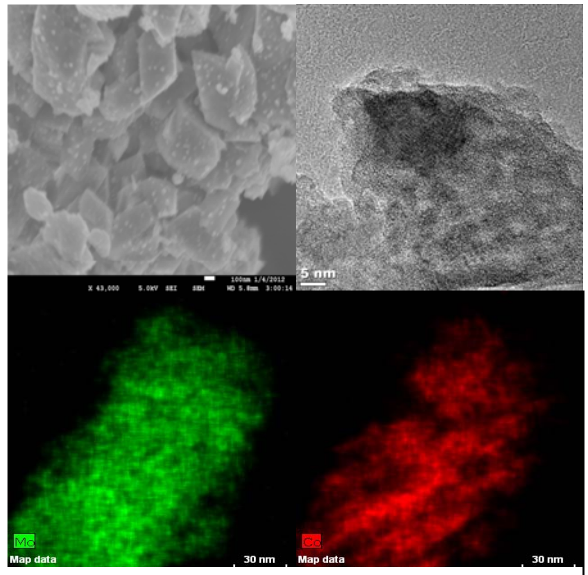
APPROACH:

While a good deal is known about the general features of oxygen reduction reactions mediated by Pt and other noble metals, exploratory work is necessary to identify transition metal oxide materials with ORR activity, and to understand the structural and electronic features that promote this activity. What is the recipe for a good ORR electrocatalyst? Our target systems will allow the incorporation of a variety of transition metals with variable oxidation states to participate in reactions, have good electrical conductivity to avoid potential losses at the electrode, and have the ability to accommodate defects which may serve as active sites for ORR reaction steps. Based on the results of the first two years of this LDRD, efforts have focused on preparing and characterizing bimetallic oxynitride and nitride samples related to the Mo_2N and MoN structure types.

TECHNICAL PROGRESS AND RESULTS:

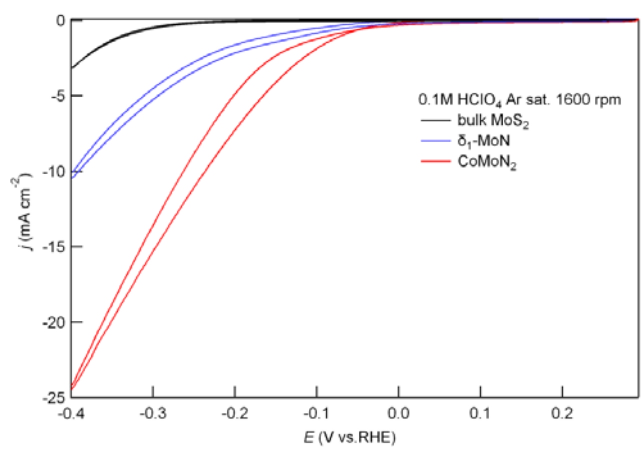
We have previously demonstrated that compounds with the nominal stoichiometry CoMoON have very good ORR activity (E_{onset} = 0.62 V vs. RHE in 0.1 M $HClO_4$; E_{onset} = 0.92 V vs. RHE in 0.1 M KOH), which under basic conditions is only 0.1 V away from the performance of Pt/C. This bimetallic system has enhanced activity relative to the isostructural end members CoO and Mo_2N. Recent efforts have been focused on understanding the true composition of this material, both from a bulk and from a local point of view. Extensive diffraction, microscopy, and spectroscopy studies have been carried out to achieve a comprehensive understanding of this system.

Powder X-ray diffraction patterns commonly show evidence for the presence of Co metal. Quantitative fitting of XANES spectra indicates that about half of the Co is external to the sample, while the remainder is integrated into the rock salt lattice. This is consistent with the variations in cell lattice parameters from X-ray diffraction experiments that occur in a composition-dependent manner. Electron microscopy studies found that even though the overall particle size was large, the lattice coherence was only about 5-10 nm and that a substantial porosity exists in samples. EELS and EDX maps collected using the aberration-corrected transmission electron microscopes at the CFN confirmed that although Co-rich regions exist, all regions containing Mo also contained Co in a manner consistent with the formation of a solid solution. Further evidence for solid solution formation was found through collaborative XPS measurements performed by colleagues at ORNL, which showed that the valence changes of Co and Mo were also most consistent with the formation of a solid solution.



a) SEM image of $Co_{0.50}Mo_{0.50}O_yN_z$ (823K) with smaller surface Co nanoparticles. b) TEM image of $Co_{0.50}Mo_{0.50}O_yN_z$ (823K). c) STEM EDX map of Mo distribution. d) STEM EDX map of Co distribution.

The compound $CoMoN_2$ also shows substantial ORR activity. This compound is even more remarkable in that it has excellent HER (hydrogen evolution reaction) activity, with almost no overpotential. This activity was even better than that of MoS_2, a widely studied catalyst for this process. A similar level of structural characterization (XAFS, TEM, SEM, XRD, XPS) has been carried out and the results are currently being analyzed. It appears that this compound appears to be free of oxygen. Intriguingly, recent neutron diffraction data suggests the presence of substantial amounts of hydrogen associated with this structure. It is not yet known if the hydrogen is incorporated into the structure or is external to the structure, but if it is the former, structural data may provide important insights into the catalytic mechanism of this class of compounds. The recently collected neutron diffraction data is being analyzed both in reciprocal space (Rietveld refinement of average structure) and in real space (pair-distribution function analysis of local structure), and there are some indications that the literature structure models for some members of the nitride and oxynitride catalyst families that we have been studying may be incorrect or incomplete..



Charge Generation and Transport in Films of Conjugated Polymers for Organic Photovoltaics BNL Part of a Collaborative NREL, BNL, LDRD

LDRD Project 10-014

John Miller and Andrew Cook

PURPOSE:

This LDRD has three principal scientific goals that will be supported by two developments in instruments and technique. These and the APPROACH sections are similar to those described a year ago. This project seeks to understand films of conjugated polymers in order to contribute to the development of high-efficiency organic photovoltaic (OPVs) devices. Specific scientific goals are:

1. Understand the nature of charge carriers (electrons and especially holes) in conjugated polymer films and determine their numbers (concentrations).
2. Measure and understand mobilities of charge carriers in polymers.
3. Measure and understand light-driven charge separation.

In addition to scientific and technical goals, an intent is to build a connection between BNL and NREL in the area of organic photovoltaics, based on complementary knowledge and capabilities at the two institutions. A BES program manager has indicated interest in providing funding for successful BNL/NREL collaboration.

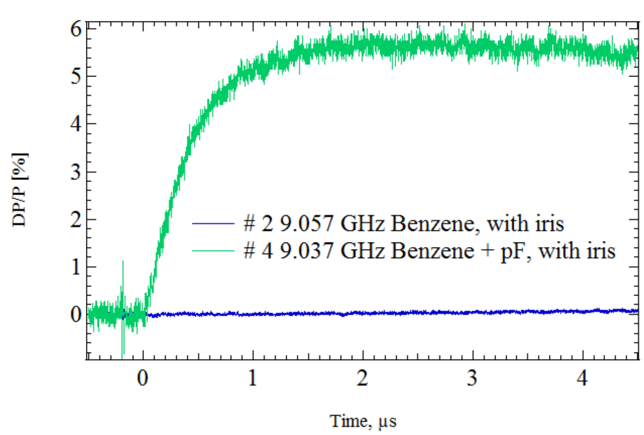
APPROACH:

To pursue these goals the two labs have developed new abilities based on the complementary capabilities and applied the instruments to the scientific goals. The instruments will include two microwave conductivity instruments. One will be an upgrade of the laser excited instrument at NREL, where it will be sited. The second, at BNL, will measure charge carriers created by 9 MeV electron pulses at BNL's Laser Electron Accelerator Facility (LEAF). This electron pulse excitation is expected to produce electron-hole pairs that have escaped the Coulomb attraction that binds them.

NREL expertise will develop methodologies to create thick (1 mm or more) films of conjugated polymers to enable spectroscopic interrogation of charge carriers created by ionizing electron pulses at LEAF. BNL expertise will develop methods to investigate the nature of the charge carriers in these thick films using, principally, optical spectroscopy, and possibly also infrared spectroscopy. An added part of the approach is to investigate infrared absorption spectroscopy as a tool for holes and electrons in conjugated polymers.

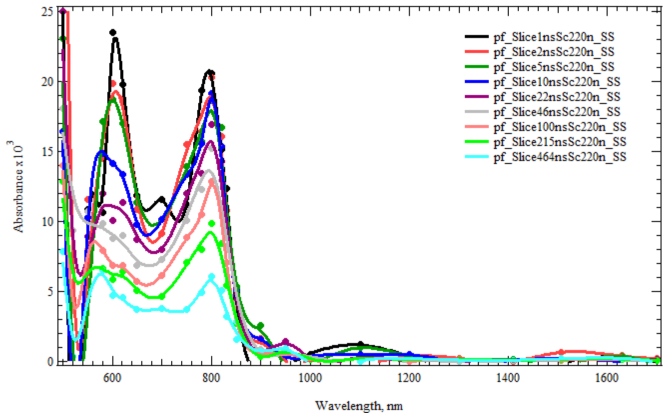
TECHNICAL PROGRESS AND RESULTS:

The two transient microwave conductivity (TRMC) instruments are operating. While much of the effort at BNL has gone into overcoming noise problems, an ongoing quest, for some experiments the instrument has operated well. Figure 1 at right shows results finding large TRMC signals from holes injected into a conjugated polymer, polyfluorene (growing green



transient) at the Van de Graaff accelerator. The blue line, without polyfluorene, shows the much smaller signal from holes with normal molecular mobilities.

Figure 2 shows an example of .partial fulfillment of the goal to examine electrons and holes in films of conjugated polymers. Thick films were created by a pressing technique and transient absorption was measured after electron pulses from the BNL's LEAF accelerator. Optical absorption spectra are shown at intervals from 1 to 463 ns. This and observations with other polymers partially fulfill our goals, however clear identification of the species responsible remains to be definitively established. Early data tentatively identifies that the principal, long-lived species may be triplet excited states.



The funding period for this LDRD is over. We and our NREL colleagues plan on more experiments over the next few months, and development of white papers for submission to BES to seek new funds.

The work will continue with support from regular program funds. Planned experiments will use trap molecules to better identify the transients. We will also attempt to overcome technical issues to enable the use of the optical fiber single-shot detection system to obtain ~20 ps time resolution, to see if charges on polymers can be clearly identified, and to understand their recombination and possible coulomb escape.

An additional theme is infrared absorption of electrons and holes in conjugated molecules. While intensities of infrared bands in molecules, expressed as molar absorption (extinction) coefficients, are typically ~200 $M^{-1}cm^{-1}$, and most bands of neutral conjugated molecules are in this range, electrons and holes give bands often 100 times stronger. The experiments, using chemical doping of conjugated oligomers and polymers, observe these intense bands, and DFT-based quantum structure calculations predict bands of similar intensities and fair, but not excellent, match for frequencies. The computed results predict differences in these bands when the polarons are paired with charged counter-ions, as they often are in chemical doping. This prediction, if correct, might provide a new method to monitor charge separation in organic photovoltaic cells.

Electrochemical Fuel Generation from Water and Carbon Dioxide

LDRD Project 10-015

James T. Muckerman

PURPOSE:

Our research focuses on efficient electrochemical water splitting and CO_2 reduction which are necessary to convert the electrical energy to hydrogen and reduced C1 compounds for fuels. Hydrogen and carbon paths can be separate (water splitting to form energy-carrying H_2; or CO_2 reduction to form energy-carrying CO or formate). Together such independent paths can produce syngas, H_2 + CO, for use in liquid fuel generation. The hydrogen and carbon paths can also be combined in CO_2 reduction directly to methanol. We are exploring the electrocatalysis of reductive half-reactions relevant to artificial photosynthesis by heterogeneous and immobilized molecular catalysts containing earth-abundant, non-noble metals.

APPROACH:

We combine experimental and theoretical approaches in closely coordinated effort to understand and improve the catalysis of fuel formation half-reactions pertinent to artificial photosynthesis. The catalysts that are the subject of our studies are both molecular transition-metal (TM) complexes and heterogeneous catalysts in the form of nanostructures, particles, films and extended surfaces. Of particular interest is the immobilization of molecular catalysts on the surfaces of electrodes or semiconductors. As part of the work on exploring new non-noble metal containing heterogeneous electrocatalysts for the hydrogen evolution reaction (HER) in acidic media, we have developed a cheaper, stable and active molybdenum-nitride based electrocatalyst for the HER. PIs other than the lead PI who contributed to this project are Kotaro Sasaki, Dmitry Polyansky, Carol Creutz and Etsuko Fujita.

TECHNICAL PROGRESS AND RESULTS:

Guided by the ‘volcano plot’ in which the activity for hydrogen evolution as a function of the M-H bond strength exhibits an ascending branch followed by a descending branch, peaking at Pt, we [JTM, K. Sasaki and W.-F. Chen (RA)] designed a material on the molecular scale combining nickel, that binds H weakly, and with molybdenum, that binds H strongly. We reported the first synthesis of NiMo nitride nanosheets on a carbon support ($NiMoN_x/C$), and demonstrated the high HER electrocatalytic activity of the resulting $NiMoN_x/C$ catalyst with low overpotential and small Tafel slope.

This success focused our research in this project on the discovery of other, even better non-noble-metal based HER electrocatalysts. Despite the superior activity and good durability of the bimetallic nitride catalyst, its synthesis requires the use of hazardous ammonia gas. We subsequently developed the synthesis of molybdenum carbide (Mo_2C) which is covalently anchored to carbon supports (carbon nanotubes and XC-72R carbon black) by a simple and environmentally friendly carburization process. High electrocatalytic performance for the HER with a low overpotential and high exchange current density was demonstrated, and was correlated with the structural and ligand effects of the anchored nanocatalysts.

Most recently, we have discovered a catalyst made from earth-abundant molybdenum and common, humble soybeans (MoSoy). This catalyst, composed of a catalytic β-Mo_2C phase and an acid-proof γ-Mo_2N phase, drives the HER with low overpotentials, and is highly durable in a corrosive acidic solution over a period exceeding 500 hours. When supported on graphene sheets, the MoSoy catalyst exhibits very fast charge transfer kinetics, and its performance rivals that of noble-metal catalysts such as Pt for hydrogen production. These findings prove that the soybean (as well as other high-protein biomass) is a useful material for the generation of catalysts incorporating an abundant transition metal, thereby challenging the exclusivity of platinum catalysts in hydrogen economics.

We consider this to have been a very successful LDRD project. It has led to two “Hot Paper” publications in prestigious journals, and another significant paper about to be submitted, two provisional patent applications and a record of invention, follow-on funding (to K. Sasaki) under the Technology Maturation program, interest on the part of the Nagarjuna Group (India) in licensing our two patents, as well as funding further development work in those areas, and finalist honors for two affiliated high school student in the Siemens Competition in Math, Science & Technology.

Structural Basis of Light Perception by Phytochrome

LDRD Project 10-016

Huilin Li

PURPOSE:

Plant and certain bacteria use light for photosynthesis and for sensing their environment as well. The protein phytochrome is a well-conserved photoreceptor responsible for sensing light at the red light range. Despite its discovery nearly half a century ago, many fundamental questions remain unanswered. A key to understanding the chemical basis of the process is the structure of phytochrome. The major challenge for the traditional structural approaches such as crystallography is that the protein is unusually large, containing over 1000 amino acids and multiple functionally distinct and dynamic domains. Cryo-electron microscopy (EM) is a powerful tool for elucidating the operational mechanism of the large biological protein complexes. Our group at BNL Biosciences Department is working on the phytochrome A, a topic of great scientific significance and of direct relevance to BNL and to the U.S. Department of Energy Basic Energy Science (BES) programs.

APPROACH:

The light sensing process relies critically on dimerization of the full-length phytochrome. Existing structural studies involve breaking the large protein into smaller pieces, and solving the structure of the fragments by X-ray crystallography. This approach is insufficient to understanding how the multiple domains dimerize and cooperate to function as a whole. Our plan is to use cryo-EM and 3-dimensional (3D) image reconstruction approaches to reveal the structure of the biologically functional phytochrome dimer.

Because phytochrome is well conserved from certain bacteria to plant (Fig. 1), the structure of bacterial phytochrome will provide initial insight into the plant system. We therefore started our investigation with the bacterial phytochrome, which is much easier to produce in a sufficient quantity (100 μg) and in a highly purified form. The second step is to study the structure of purified plant phytochrome. In the longer term, we plan to reveal the conformational changes of the bacterial and plant phytochrome between red and far-red states. The latter is a highly challenging task. We collaborate with plant biologist Dr. Richard Vierstra at the University of Wisconsin.

TECHNICAL PROGRESS AND RESULTS:

During the first funding year 2010, we worked on the bacterial system, specifically, the bacteriophytochrome from *Deinococcus radiodurans* (DrBphP). We obtained the cryo-EM structure to a resolution at which individual domains of the DrBphP dimer are resolved as different densities. This level of detail in the structure enabled us to computationally "dock" into the 3D density map with several published crystal structures of the fragments of homologous bacteriophytochrome.

Our cryo-EM studies revealed that, contrary to the long-standing view that the two monomers are held together solely via their carboxyl terminal region, we found that the amino terminal bilin-binding region of BphP also provides a dimerization interface with the C-terminal kinase domain appearing as a more flexible appendage. The BphP monomers were found to dimerize in

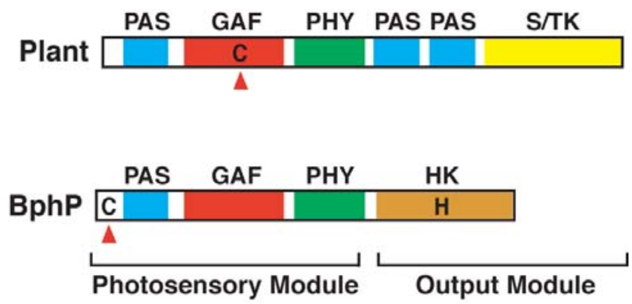


Figure 1. A comparison of the domain organization of the plant PhyA with the bacterial phytochrome BphP. Note the two additional PAS domains preceding the S/T kinase domain in the plant PhyA.

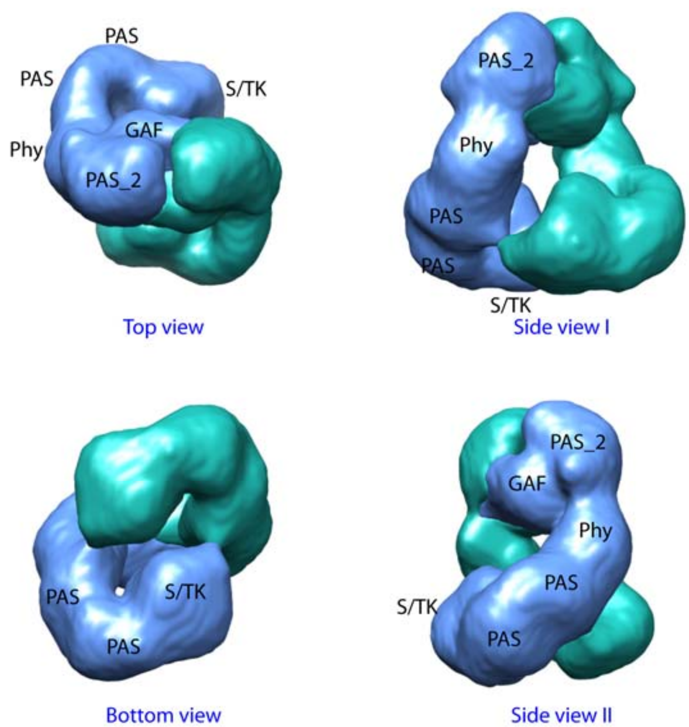


Figure 2. The 3D map of the plant *Arabidopsis thaliana* phytochrome-A dimer as determined by three-dimensional image reconstruction from electron microscopy images. The two monomers making up the complete dimer structure are shown in blue and cyan respectively. The individual domains of the protein are labeled. The AtPhyA apparently dimerizes in parallel with the two polypeptides intimately twisting around each other, particularly at both N and C-terminal ends, leaving a large gap in the middle region.

parallel with the polypeptides intimately twisting around each other in a right-handed fashion. The DrBphP work was published in Proc. Natl. Acad. Sci. USA in 2010.

During fiscal years 2011 and 2012, we focused on the plant phytochrome A system, the *Arabidopsis thaliana* PhyA (AtPhyA). We have obtained highly purified PhyA sample. We also found good conditions to prepare the EM grids of the plant PhyA, which produced well-contrasted EM images. We have collected a large dataset and most recently, we have obtained the 3D reconstruction of AtPhyA. We are mapping the 3D density with a number of strategies including antibody labeling and protein fusion methods. When this part of the work is done, we plan to dock the 3D EM map with the homolog crystallographic domain structures. We will then compare this plant structure with the bacterial version, in order to find out how similarly or differently these two evolutionary related chromo-proteins function. We plan to write a paper to report this research.

Our longer-term goal is to study the structural dynamics of PhyA at the different light absorption states.

New Model Organisms for Analysis of Plant Metabolism

LDRD Project 10-017
Jorg Schwender

PURPOSE:

The objective of this LDRD proposal is to establish expertise at BNL in new model plants which have relevance as energy crops that can undergo metabolic engineering and flux analysis approaches. Transgenic lines which are affected in the synthesis of storage products will be produced and their central metabolism studied by flux analysis of developing seeds. A future target of funding will be the establishment of a Bioenergy Institute linking genetics/genomics expertise at Cold Spring Harbor Laboratory (led by Dr. R. Martienssen) with expertise in metabolic engineering and flux analysis of Shanklin/Schwender at BNL. Therefore support of this project will foster improved integration of BNL's BES-supported groups (Schwender, Shanklin) as encouraged by our Program Managers.

APPROACH:

Criteria for selection of model plants are short generation time, self pollination, suitability for genetic transformation, high sequence homology between genes of the new model plant and other well established model plants (*Arabidopsis*), and low complexity and size of the genome. For the purpose of studying seed metabolism by flux analysis, seeds must be of sufficient size. Developing embryos at an early stage of development will be dissected out of seeds under aseptic conditions and put into a synthetic liquid culture medium containing different organic substrates. The composition of storage compounds (oil, protein, starch) after culture should be similar between cultured embryos and seeds that matured in plants.

TECHNICAL PROGRESS AND RESULTS:

We obtained seeds of Field Pennycress (*Thlaspi arvense)* from the Arabidopsis Biological Resource Center and determined the following growth characteristics: Growth from seedling to flowering 4.5 – 5.5 weeks; ca. 7.5 weeks until developing embryos can be dissected out of seeds for cultures. Weight per seed ca. 1.0 – 1.3 mg. 300 – 900 seeds produced per plant. To establish *in vitro* culture conditions we dissected early-stage embryos out of developing seeds and grew them in liquid culture medium under continuous light. The liquid medium was adapted from former studies with similar plant species (*Brassica napus*). The embryos grew continuously in culture up to 20 days and the final biomass composition was similar to that of mature seeds (Fig. 1).

The *in vitro* culture system was now used in combination with an isotopic tracer (^{13}C-labeled glucose) to study metabolic flux under the established controlled culture environment. Embryos were cultured for 10 days and then harvested. Extraction and fractionation of the embryo tissue ($CHCl_3$/Methanol/H_2O) was followed by further hydrolysis of biomass polymers according to our standard protocols. Finally 130 mass isotopomer fractions were quantified in protein derived amino acids, fatty acids, starch, and free sucrose by Gas Chromatography / Mass Spectrometry. These data are later to be used to derive a flux map of central metabolism.

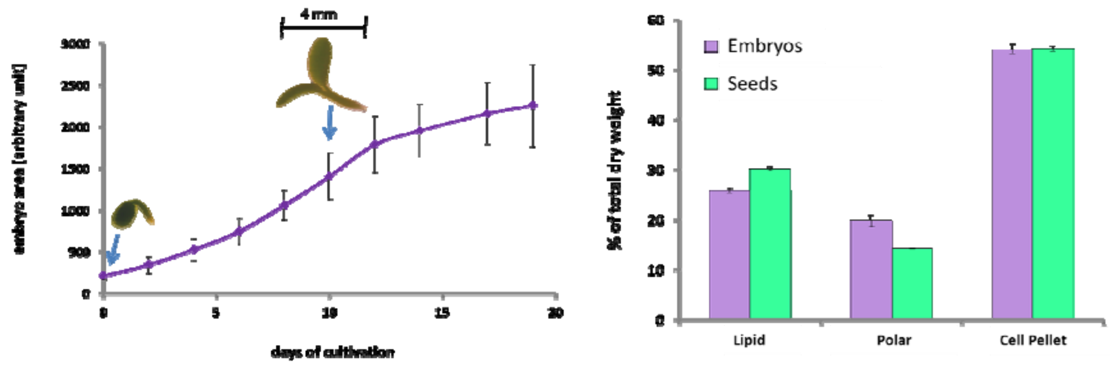


Fig. 1: Growth of embryos of wild-type pennycress in liquid culture under conditions used for labeling experiments. As a measure of embryo size, the surface area was determined using a LemnaTec Imaging System (LemnaTec GmbH; Wuerselen, Germany) (area of embryo ± SD; n=35). Fractions of major biomass compounds in cultivated embryos and in mature seeds relative to total dry weights (% of total dry weight ± SD; n=4).

In order to demonstrate that our model plant can be genetically transformed, we generated two genetic constructs. *A. thaliana* cDNAs for the WRINKLED1 transcription factor (AtWri1, At3g54320) and the plastidic isoform of NADP-malic enzyme (NADP-ME4, At1g79750) were cloned into the vector pDs-Red-35S carrying a DsRed fluorescent selectable marker and the constitutive cauliflower mosaic virus (CaMV) 35S promoter. *Agrobacterium* mediated transformation (floral dip method) in *T. arvense* was successful and resulted in multiple lines constitutively overexpressing AtWRINKLED1 and AtNADP-ME4. Both transgenic modifications relate to the formation of plastidic pyruvate, the precursor of fatty acid synthesis in plastids during oil synthesis and therefore will be useful to explore the modification of oil content in seeds by ^{13}C-Metabolic Flux Analysis.

To study metabolic flux in *T. arvense* developing seeds, the metabolic network must be defined. Therefore we performed transcript profiling for cultured developing embryos of *T. arvense*. In collaboration with the group of Dr. R. Martienssen, Illumina deep sequencing of the transcriptome was obtained. About 100 million short read sequences were assembled into long contiguous RNA sequences (contigs) by using high performance computational resources at BNL. This resulted in a high quality comprehensive transcriptome of developing embryos. Sequence alignment of the *T. arvense* transcripts to the *Arabidopsis* predicted proteome by translated BLAST database search revealed a high sequence homology to *Arabidopsis thaliana* encoded gene transcripts, mostly > 90% identity in amino acid sequence. This transcriptome information will allow identifying all relevant genes in central metabolism and the assessment of their expression levels in developing seeds of *T. arvense*.

Further sequence analysis of the transcriptome also suggests that single copy genes of *Arabidopsis* typically have only one ortholog in *T. arvense*. This means that our *T. arvense* accession most likely has a simple diploid genome, which is very advantageous for future genetic studies. We confirmed the genomic organization independently. In collaboration with Dr. Steffen Hameister (Institute of Botany, University of Natural Resources and Life Sciences, Vienna) we determined the genome size of *T. arvense* based on DNA flow cytometry. The C-value of 0.48 – 0.49 is similar to the value obtained before for another *T. arvense* accession (1C = 0.52 pg), which had been reported to be diploid with *n* = 14 chromosomes (Lysak et al., 2009, Molecular Biology and Evolution 26: 85-98).

Having established *T. arvense* to be suitable for *in-vitro* embryo culture and metabolic flux analysis of developing seeds, amenable to genetic transformation, and having determined the transcriptome as well as the genome organization, we will be using this organism in future studies funded by DOE.

Development of Large Liquid Argon Time Projection Chambers (LArTPC) for Future Neutrino Experiments

LDRD Project 10-025

F. Lanni, Y. Li, B. Morse, H. Themann, C. Thorn

PURPOSE:

Liquid argon (LAr) has been successfully used in many high energy particle calorimeters since it was first proposed at BNL in 1974. More recently, there has been a growing effort to develop giant LAr Time Projection Chambers (TPCs) as an alternative to Water Cerenkov Detectors for neutrino physics measurements. In order to develop and optimize LAr TPCs to exploit their high resolution 3D imaging and energy measuring capabilities, all of the physical processes that produce and transport charge and light signals in LAr must be quantitatively understood. Much engineering information is available (small LAr TPCs have been built) but scaling to future multi-kiloton detectors requires basic property determination with high precision data. This project will measure the fundamental properties of charge and light production and transport in LAr, investigate and optimize designs of devices and structures for charge and light collection, and develop the operation of electronics systems in LAr. The ultimate result of this project will be the knowledge to successfully construct a 100–kiloton scale LAr TPC for neutrino physics and proton decay experiments.

APPROACH:

We emphasize the fundamental physics and electronics that must be understood and applied to design the next generation of noble liquid TPCs. Basic properties of noble liquids are known only incompletely, and electronic systems optimized for operation in very large cryogenic detectors have not yet been developed. Aspects of the program include these:
Create the infrastructure for cryogenic measurements:

- Construction of cryostats to contain the noble fluids, recirculating purification systems to achieve and maintain high fluid purity, and the required instrumentation.

Measure basic noble liquid transport properties:

- Diffusion of electrons, electron attachment to impurities and electron-ion recombination will be measured to understand charge transport and production. Use of additives dissolved in the noble liquid to enhance charge or light production will be explored.
- Quantitative measurements of the partition of impurities between the liquid and gas phase of noble liquids and of the kinetics of impurity generation and transport will be measured.

Readout electronics development:

- For truly large detectors it will not be feasible to have one cable and cryogenic feed-through per readout channel. The entire signal processing chain through digitization and multiplexing must therefore operate in the noble liquid at cryogenic temperatures. This will de done by designing and fabricating analog and digital CMOS ASICs for cryogenic operation. The objective is to reduce the entire electronics system and the TPC structure to modules that are arrayed to scale to any detector volume or shape.
- Modeling and measurement of the entire signal formation process, for both charge and light, using measurements of the basic transport properties described above.

TECHNICAL PROGRESS AND RESULTS:

1. We have established a cryogenics lab for liquid noble fluid R&D. A postdoc (Yichen Li) has been hired to plan and execute the experiments. A 0.3 m^3 cryostat has been instrumented to evaluate electronics performance and reliability in LAr, and has been successfully evaluating the performance and lifetime of commercial voltage regulators for the past year. A small cryostat and purification system was designed, fabricated and assembled, for photocathode quantum efficiency and electron diffusion measurements in ultra-high purity LAr.

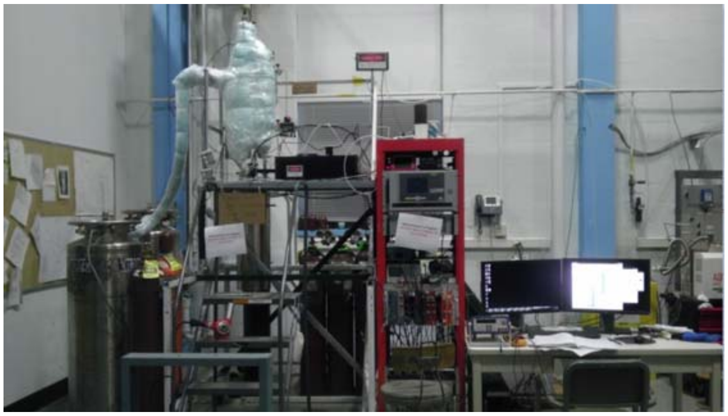


Figure 1: The experimental system running under cryogenic temperature.

2. During September 2012 we had a run with gaseous Argon under room temperature after we passed the cryogenic safety review which is important for the startup of the measurement. The performance of the electronics, DAQ and optical system satisfied the expectations during the operation. The quantum efficiency of the Au photocathode was measured in gaseous Argon as ~10^{-8}-10^{-7}. The electron drift and longitudinal diffusion as a function of drift field were also measured in the gaseous argon, and the results agree with the previous measurements.

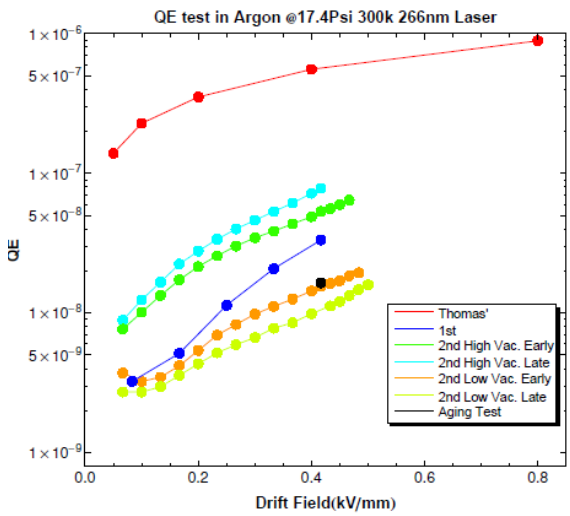


Figure 2: The quantum efficiency of Au photocathode in gaseous Argon.

3. Late 2012 we had an engineering run with liquid Argon under cryogenic temperature ~83K. The setup is shown in Figure 1. The performance of the control and purification system was testified under the cryogenic condition. The purity level of liquid Argon was monitored and significantly improved compared to the room temperature results attributing the low temperature. During the cryogenic run, several engineering problems were discovered and fixed. The first liquid Argon physics run is planned for February 2013.

Spin Waves in Artificial Magnonic Crystals: Fabrication, Imaging and Scattering

LDRD Project 10-034
Dr. Darío Arena, PSD; Peter Warnicke, PSD
Co-PI(s): Dr. Aaron Stein, CFN and Dr. Yimei Zhu, CMPMSD

PURPOSE:

Spintronics, where the electron's spin in addition to its charge is central to the operation of the device, is one possible replacement for CMOS electronics based on silicon. A subset of spintronics, spin wave (SW) electronics, holds great promise in moving into the post-CMOS era. SW electronics may also play a part in reducing energy consumption as their function derives from the propagation of spin, not charge, and hence there is little energy loss from Ohmic heating. The propagation and manipulation of SWs can be examined in lithographically-defined magnonic crystals (MCs), where now, instead of electromagnetic waves, the relevant excitations are spin waves, quantized as *magnons*, which are collective excitations of the spins of valence electrons in a ferromagnet (FM). In this LDRD, we have been utilizing the advanced lithography tools available at the CFN (in collaboration with Dr. Aaron Stein) to fabricate MCs. In addition, we have set up a laboratory to characterize their high-frequency (GHz range) properties. Also, we have been collaborating with Dr. Yimei Zhu at CMPMSD to eventually investigate the excitations in MCs using advanced TEM imaging. Lastly, we have been extending our ultrafast, x-ray-based spectroscopy to examine the excitations of the MCs, which we will investigate using x-ray microscopy. The techniques at these non-BNL facilities (x-ray microscopy, ultrafast time-resolved x-ray scattering) may be developed at NSLS-II.

APPROACH:

The program supported under this LDRD project consists of several tasks: (1) fabrication of MCs at the CFN; (2) characterization of the microwave excitation spectra of the MCs using ferromagnetic resonance utilizing a vector network analyzer (VNA); (3) examination of the SW standing wave patterns using Lorentz TEM microscopy; (4) measurement of x-ray scattering patterns of SWs in MCs; (5) imaging of SWs in MCs using x-ray microscopy. Task 1 will be conducted primarily at the CFN. Task 2 will be performed at the NSLS using equipment purchased for this purpose under the LDRD program. Task 3 will be carried out at BNL in collaboration with Dr. Yimei Zhu. Task 4 will be executed at NSLS at beam line U4B, although access to more advanced facilities at 3rd generation storage rings may be required. Task 5 will be carried out at the XM-1 soft x-ray, full-field transmission microscope at the ALS at LBNL.

TECHNICAL PROGRESS AND RESULTS:

In FY12, the LDRD funding lasted for the 1st quarter of the fiscal year. Hence, the LDRD-related activities focused on completing measurements and preparation of publications. To date, two publications have resulted from the LDRD (see list at bottom). In reference [1], we explore the use of soft x-ray microscopy for imaging of nanometer magnetic films very similar to the films that will be used in the studies of MCs, this case a multilayer magnetic film where the active magnetic layers are: |10 $Fe_{19}Ni_{81}$ |10 Cu | [0.2 Co | 0.6 Ni] x n | 0.2 Co |. The numbers indicate the thickness of the layers in nm, and the integer n indicates the number of repeats in the Co-Ni layers. Hence, for n = 4, the total cobalt thickness is only 1.0 nm. The Fe-Ni layer has an in-plane magnetic easy axis, while the repeated interfaces in the Co-Ni layer produce a composite layer with an out-of-plane magnetic easy axis. Films with this hybrid anisotropy are currently under extensive investigation as they may

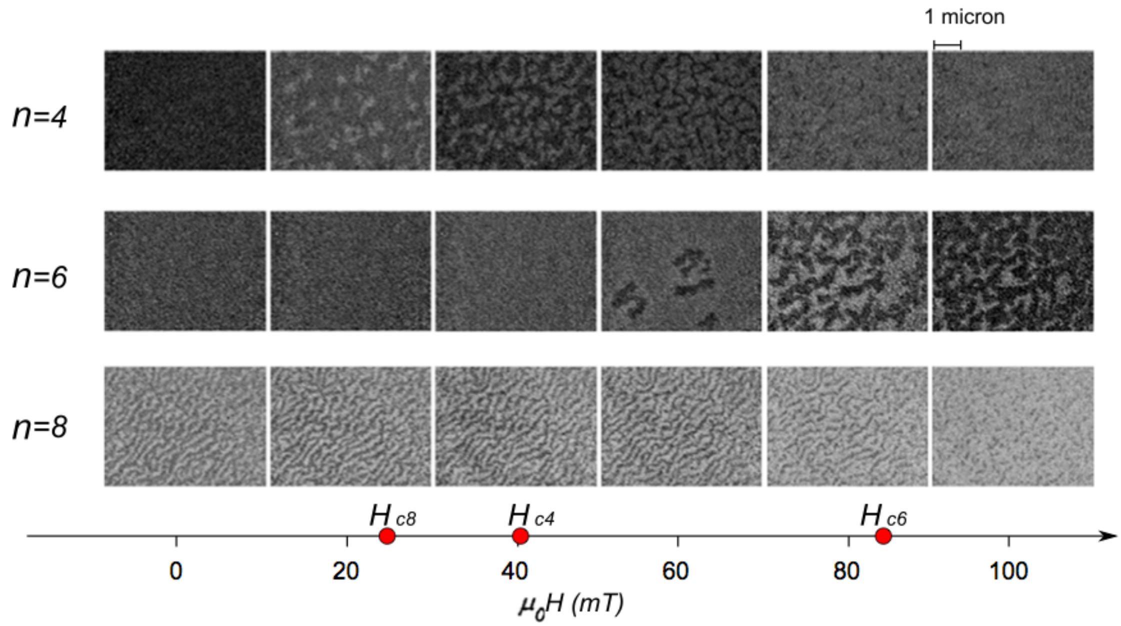


Image from Ref. [1] showing the evolution of the magnetic domain pattern in Ni/Co multilayer films, acquired using the XM-1 microscope at the Advanced Light Source. The images were generated by tuning the x-ray energy to the cobalt L_3 edge. The integers on the left indicate the number of repeats in the Co/Ni structure, and the n=4 has an equivalent total cobalt thickness of 1 nm. The clear domain pattern visible for this sample establishes a new lower bound on the sensitivitv of the XM-1 instrument.

improve the properties of nanoscale spin-torque nano-oscillators (STNOs), which are emitters of spin waves and can be used as point sources of spin waves injected into MCs. A main finding of the manuscript is that a clear magnetic domain pattern can be observed for even the $n = 4$ repeats Co-Ni sample, which establishes a new record for magnetic sensitivity at the XM-1 microscope.

In manuscript [2], which was recently accepted for publication in *Journal of Applied Physics*, we investigated the limits of x-ray detected ferromagnetic resonance (X-FMR), which is a key component in exciting spin-wave modes in MCs while simultaneously exploring their properties with x-rays. In this article, we undertook X-FMR measurements at the MAX-II synchrotron in Lund, Sweden. The key finding in this article is that even though the x-ray bunch length at MAX-II is about 400 ps, implying a Nyquist sampling limit for oscillatory motion of around 1.25 GHz, we were able to extract an oscillatory signal up to 2.5 GHz. In addition, we developed an analytical model for retrieving signals in X-FMR measurements, taking into account issues such as x-ray bunch length, timing jitter, and driving frequency. The results and analysis presented in the article provide support for using newer synchrotron facilities, such as NSLS-II, which will have an x-ray bunch length of approximately 45 ps, to extend the frequency range of X-FMR measurements even further, beyond 10 GHz and, in special operating modes, even towards 50 GHz and beyond.

[1] F. Macia, P. Warnicke, D. Bedau, M.Y. Im, P. Fischer, D.A Arena, A.D. Kent “Perpendicular magnetic anisotropy in ultrathin Co— Ni multilayer films studied with ferromagnetic resonance and magnetic x-ray microspectroscopy,” *Journal of Magnetism and Magnetic Materials*, **324** (22) 3629-3632 (2012).

[2] P. Warnicke, R. Knut, E. Wahlstrom, O. Karis, W. E. Bailey, and D. A. Arena, “Exploring the accessible frequency range of phase-resolved ferromagnetic resonance detected with x-rays,” *Journal of Applied Physics* **113**, 033904 (2013).

EIC Polarized Electron Gun

LDRD Project 10-039

Ilan Ben-Zvi

PURPOSE:

The eRHIC project requires a highly polarized electron source with high average current, which sounds ambitious based on state-of-the-art polarized electron source technology. Average current of about 4 mA of polarized electron beam has been obtained in Jefferson Lab. But eRHIC requires 50 mA of average current. There are other requirements which make the source more challenging: final transverse emittance, one of the most important parameters describing beam's quality, needs to be less than 20 mm.mrad; bunch charge should be about 3.5 nC; final bunch length should be less than 4 mm. A natural way of obtaining the 50 mA of average current is to employ multiple cathodes, up to 20 cathodes, and combine the beam bunches from each cathode together to form one bunched beam. It works like a "Gatling gun". With funneling, any improvement applied to single polarized sources will multiply the performance of the funneled source. In this study we will try to prove that funneling works for polarized electron sources in a geometry and capabilities that are suitable for the future eRHIC (polarized electron collider addition to the RHIC heavy ion collider).

APPROACH:

A critical requirement for a photo cathode to achieve a high polarized electron current for an extended period is the ability to maintain an extreme high vacuum (XHV) level of 10^{-12} Torr. It is essential to establish this condition during cathode fabrication, storage and operation. Due to the complex geometry and surface properties of a vacuum chamber capable of supporting 20 cathodes, it is essential to establish the full scale gun geometry in order to demonstrate cathode performance under prerequisite levels of vacuum and voltages levels. We plan to first demonstrate performance using a minimum of 2 cathodes.

We are establishing the preparation of GaAs cathode manufacturing as well as all the essential components of the Gatling Gun vacuum system here at BNL. Addressed are the design and construction of a cathode preparation system at BNL and all the main components of the Gun and of the two main elements, the cathode preparation system and the gun chamber, compatible with XHV vacuum while providing for the frequent replacement of the cathode. Another issue is the design of the combiner that can merge individual beam-lets from 20 cathodes without degrading the quality of the electron beam. Other investigators are: Vladimir Litvinenko, Alexander Pikin, Triveni Rao, Brian Sheehy, John Skaritka, Omer Rahman, Eric Riehn, Qiong Wu, Erdong Wang.

TECHNICAL PROGRESS AND RESULTS:

A review of the Gatling Gun program was performed by an international committee in June 2012. Reviewer comments note that though the goals of the Gatling Gun program are ambitious, the program is well organized, all critical developmental issues are being adequately addressed and the development is proceeding well, commensurate with available resources.

A detailed high-resolution electrostatic simulation of the gun was carried out. The simulation led to some modification of the electrodes of the gun and improved peak surface electric fields. The depressed-collector design has been carried out. A detailed 3-D beam dynamics simulation with space-charge was carried out, refining and confirming the initial 2-D calculations. Polarized cathode activation was done and measurements were carried out in the activation chamber that was delivered earlier this year. The components of the gun made great progress, and delivery of all components will take place in 2013 (see more details below).

<u>In fiscal year 2012 we have finished the following:</u>

1. Detailed electrostatic modeling of the main gun chamber.
2. Design of the depressed-collector.
3. Detailed 3-D beam dynamics modeling with space-charge.
4. Mechanical design manufacturing of all components for the main gun chamber.
5. Procurement and successful testing of 250kV power supply.
6. Manufacturing and testing of the high voltage feed through .
7. Manufacturing of the first bend dipoles for 2 beam operation.
8. Design of the funneling (combiner) magnet.
9. A cathode preparation system was manufactured and assembled in building 966.
10. A vacuum in the range of 10^{-12}Torr was successfully demonstrated in the Grand Central vessel. This is the largest known chamber that has achieved XHV operation in industry.
11. XHV vacuum procedures have been established at BNL and 10^{-12}Torr vacuum levels can now be routinely demonstrated in the cathode preparation system.
12. Cathode shroud assembly manufacturing has been completed.
13. Cathode cooling ring has been completed and integrated into the cathode shroud assembly.
14. Focusing solenoids have been completed and integrated into the Anode assembly.
15. The Anode Sub-assembly has been completed and the system leak checked.

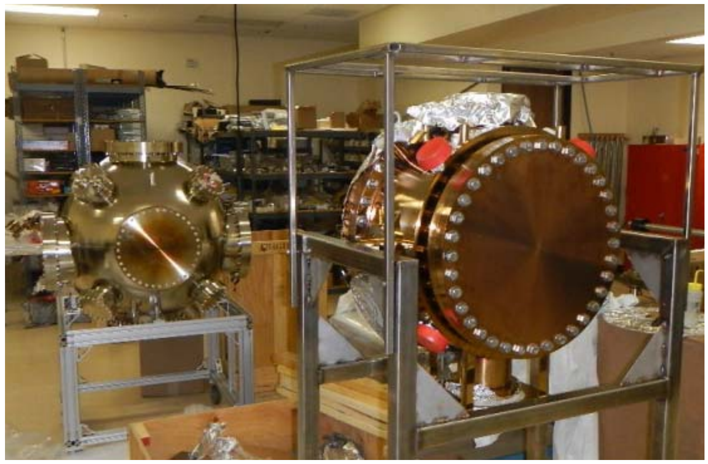
<u>Present status of the project:</u>

Post-doc (Eric Riehn) and graduate student (Omer Rahman) are refining the detailed design and testing the cathode preparation system to manufacture the cathodes for use in the first gun test.
Gun Vessel is under XHV testing at the system integrator Transfer Engineering.
Gun manipulators - components are being integrated into the main vessel and will undergo XHV testing at the manufacturer.
Activation chamber manipulators - component integration is underway at the manufacturer.
Gun end transition Assembly - component subassembly integration has begun at the manufacturer.
Cathode Shroud Assembly - has been sent for high pressure rinse (HPR) with ultrahigh purity water to minimize cathode surface field emission.
Alumina Combiner Break - remanufacturing has been successfully completed and is being leak checked at the Atlas Company.
A high voltage and laser safety enclosure is being manufactured in preparation for system performance testing at BNL.

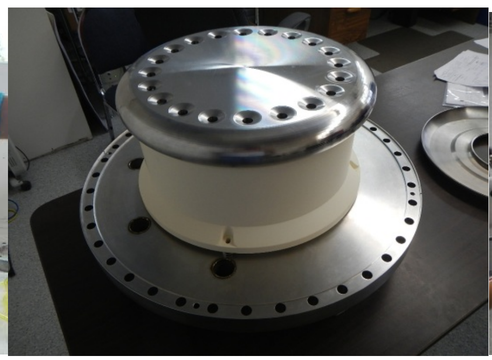
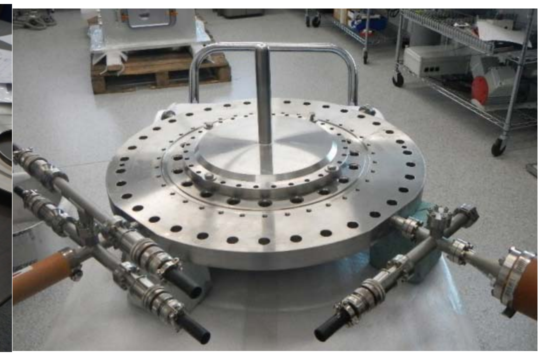
MILESTONES FOR FY13:

Gatling Gun vacuum system integrated and vacuum tested…...4/2013
HV testing of completed Gatling Gun and XHV tested……… 5/2013
Gun Cathodes routinely produced in single prep system...........6/2013
High voltage safety enclosure completed and tested…………..7/2013
Phase 1 Combiner tested and installed………………………...8/2013
One and Two Cathode operation …………….………..……….....9/2013

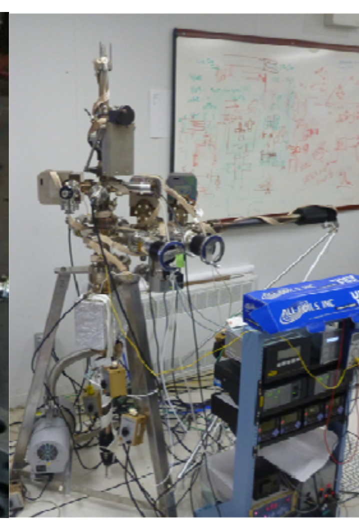
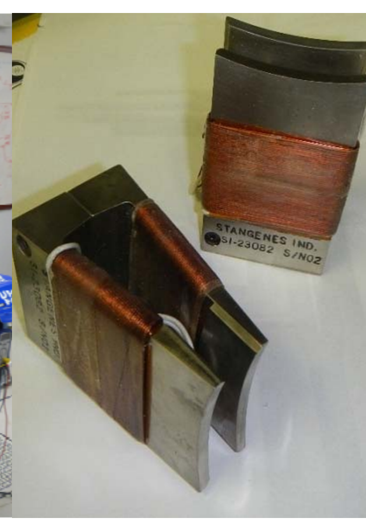
Figures from left to right: Cathode preparation chamber during and after XHV tests, Main Gun Chamber and 250 kV power


20 Cathode 316L stainless steel shroud after polishing, cathode shroud assembly. on 27” wire seal flange and transition end of anode assembly

Multi-port titanium anode, BNL Gun cathode preparation system, first bend dipole magnets, Ceramic tube for funneling (combiner) section.

Development of a Laser System for Driving the Photocathode of the Polarized Electron Source for the EIC

LDRD Project 10-040

T. Rao, T. Tsang, B. Sheehy

PURPOSE:

The objectives of the project are the development of the laser system that can drive a single cathode and improvement in the performance of the cathode of the “Gatling Gun”. The laser should be upgradable to deliver the 50 mA current required for the electron-ion collider (EIC) with appropriate timing and energy stability. In this project, three different laser systems will be investigated, and an appropriate system will be chosen and developed. The improvement in the sensitivity of the cathode is achieved by better understanding of the formation of the negative electron affinity surface. Different oxygen sources for creating the negative electron affinity surface as well as the changes in the surface morphology as a function of the cleaning temperature will be investigated. Polarized electron source (cathode and laser) capable of delivering up to 50 mA with life time significantly longer than its preparation time is crucial for the eRHIC project at BNL

APPROACH:

The quantum efficiency (QE) of the polarized electron source is in the range of a fraction of a percent at 780 nm. In order to meet the beam requirements of the Gatling gun, the laser should deliver ~ 4 W average power at 780 nm, at a repetition rate of 704 kHz with a pulse duration of ~ 1 ns at each of the gun cathodes. Formation of the negative electron affinity surface on the GaAs is crucial for the high QE, and the preservation of the polarization. Typically the electron affinity of a very clean GaAs surface is reduced by depositing Cs and an oxidizing agent to result in a fractional monolayer of Cs on the surface. The cleanliness of the GaAs surface, Cs and the oxidizing agent determine the ultimate QE of the cathode and its sensitivity.

The scope of the program is expanded to address both the development of the laser system and the understanding the negative electron affinity of the cathode in order to increase the life time of the cathode. In collaboration with Brian Sheehy of C-AD, we investigated different laser architectures, decided on the most promising design, interfaced with industry to complete the preliminary research and development and initiated the procurement process for the laser system. Experiments to establish the correlation between the QE and the surface properties of GaAs upon heating have been completed. The results indicate that when normalized to the initial QE, the temperature of the substrate during heat cleaning does not affect the final QE as long as the substrate is heated above 560 C. The vacuum system is being modified to accommodate activation using two alkali metals instead of one to decrease the sensitivity of the cathode to contaminants.

TECHNICAL PROGRESS AND RESULTS:

The fiber laser system operating at 1560 nm has been developed by Optilab, a commercial firm. Using pulses from a function generator with a repetition rate of 352 kHz and pulse duration of 2.4 ns, an average power of > 10 W and peak power of > 13 kW has been extracted from this device at Optilab’s facility. The laser was damaged during a pre-acceptance test at the vendor’s facility and had to be repaired. The repair appeared to be successful, but after delivery to

Brookhaven, acceptance testing revealed that there were problems with the laser performance at high power. One of the challenges of such a fiber laser is managing the onset and growth of nonlinear effects with increasing power. These effects result in gain going to longer wavelengths at the expense of the desired laser line. Thus the peak power in the 1560 nm line was being clamped between 1 and 2 kilowatts, instead of the 10 kW target. This can be seen in the logarithmic plot below, which shows the evolution of the laser amplifier spectrum as the power is progressively increased: the long-wavelength tail grows rapidly as the pump current (Drv1 in the figure) and output power (indicated in the legend) are increased. This problem may have arisen during the repair that followed the failure in the pre-acceptance test. The laser has been returned to Optilab to repair this problem.

Optilab was unable to complete the frequency-doubling component of the laser project. We have identified another vendor capable of constructing it, but wish to wait until we can completely characterize the 1560 nm laser before issuing that contract. Depending on the timing, we may just construct the doubler here at BNL from components.

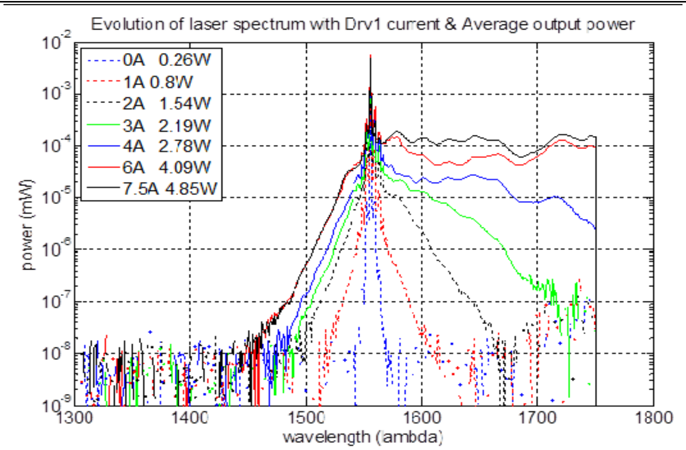


Figure 1 Evolution of 1560 nm spectrum showing the onset and growth of nonlinear effects in the fiber laser, which can be seen in the rising long-wavelength component. The power indicated in the y-axis is measured after large attenuation and should be regarded here as in relative units.

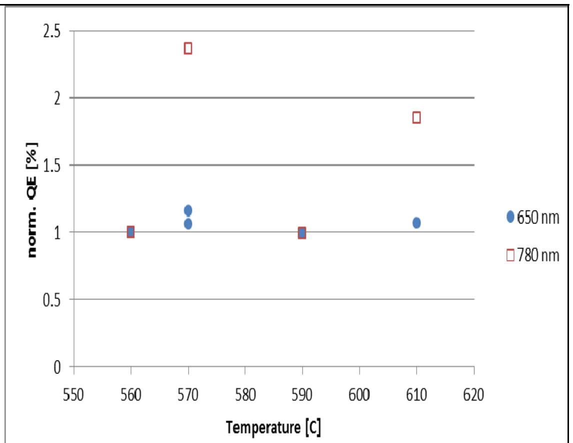


Figure 2 Normalized QE as a function of cleaning temperature at 650 and 780 nm. The variation in QE for 780 nm is attributed to the spatial variation

In order to correlate the cleaning temperature to the QE, QE (defined as QE initial) of a number of samples from the same wafer were measured at 650 nm and 780 nm after heating it to 560 C and activating it. Each of the samples was then heated to temperatures ranging from 560 C to 610 C. The QE of each sample (defined as QE temp.) was measured after heating at a higher temperature and activation. Figure 2 illustrates that (QE temp/QE initial) does not depend on the cleaning temperature.

2013 Milestones:

Install and characterize the laser system
Correlate QE of the cathode to its surface morphology
Investigate the life time of the cathode with dual alkali activation

Simulation, Design, and Prototyping of an FEL for Proof-of-Principle of Coherent Electron Cooling

LDRD Project 10-041

Vladimir N Litvinenko

PURPOSE:

Free-electron laser (FEL)-based Coherent Electron Cooling [1] (CeC) promises to become a revolutionary method that will significantly increase luminosity in proton-proton colliders, ranging from RHIC to the LHC. We are addressing issues, theoretical and numerical, that the FEL community has put aside for at least two decades. We are modifying the well-benchmarked 3D FEL codes specifically for the CeC cooler. It is very unlikely that we can readily employ existing wiggler designs with their very small gaps suited for light sources and short wavelength FELs. Accordingly, we are designing and fabricating a prototype of such a wiggler to address possible shortcomings and limitations. This LDRD is the front-runner project for testing the CeC mechanism in a proof-of-principle (PoP) experiment. With the success of the CeC PoP, the CeC cooler certainly will greatly benefit future medium- and full-energy eRHICs. Importantly, it will ensure that we maintain our competitive edge against EIC projects, such as the ELIC.

APPROACH:

The theoretical part of our research focuses on the evolution of the e-beam phase-space distribution in the FEL with arbitrary initial conditions and under the influence of space charge. This fiscal year we had focused on analytical solutions for an electron beam with finite size, which is a very nontrivial fit. We address the following theoretical and design challenges:

1. Designing the CeC PoP experiment and placing orders for main long lead items 9SRF accelerator cavities and cryogenic systems;

2. Simulating CeC's performance for a realistic beam and lattice; and,

3. Testing prototype of the helical wiggler. The CeC PoP experiment requires a new helical wiggler, suitable for installing into RHIC's Interaction Point between two DX magnets. It should have an aperture adequate to avoid imposing any constraints on the RHIC's hadron beam. Using these LDRD funds, a short prototype of such a wiggler had been built and its magnetic filed had been measured. The performance of the wiggler was well within the specs.

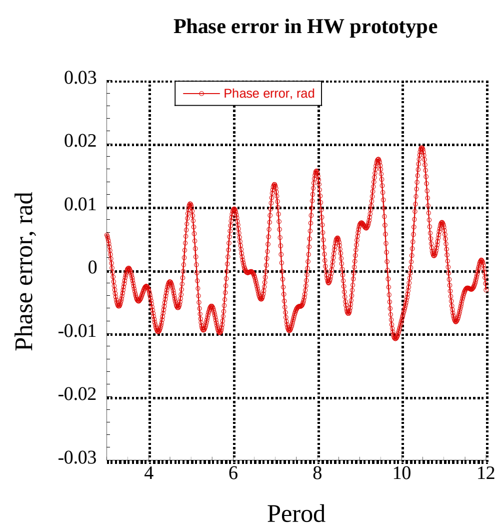
TECHNICAL PROGRESS AND RESULTS:

During this fiscal year we developed detailed design of the CeC experiment– see Fig. 1 [4, 5]. We also achieved significant progress both in the theory and computer simulations of the processes in coherent electron cooler [2-16]. The main theoretical accomplishments are discovery of the beam-conditioning for the CeC process [6] and rigorous proof that there is only a single growing mode in the FEL [2-3].

Fig. 1. Layout of the CeC PoP experiment.

On the experimental side there is significant progress in design and manufacturing of major parts of the CeC experiment, including 50 cm prototype of helical wiggler, which is paid for by this project's funds. Budker Institute of Nuclear Physics (BINP Novosibirsk, Russia) had finished the prototyping and evaluations of the prototype. This task was the only unfinished part of this LDRD proposal. The final report, expected from BINP in January 2013, and providing the remaining payments for this prototype will successfully conclude this LDRD project.

(a)



(b)

Fig. 2. Left (a) shows the 0.5 m helical wiggler prototype undergoing magnetic measurements (b) Measured FEL phase error.

We published two refereed and thirteen conference proceeding paper on the subject of coherent electron cooling during reporting period. We also were awarded FY12 $1.28 funds from NP DoE competitive accelerator R&D program for experimental demonstration of coherent electron cooling and secured $0.78M for FY13. Our early start with LDRD funds in prototyping the wiggler for CeC was of critical importance for this success. Successful completion of the wiggler prototyping will allow us to place order for full CeC wiggler early in 2013.

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Realization of an e+A Physics Event Generator for the EIC

LDRD Project 10-042

Thomas Ullrich and Raju Venugopalan

PURPOSE:

The prospects for a future Electron-Ion Collider (EIC) are closely tied to the strength of the physics case for an *e*A physics program at such a facility. Many of the key measurements that provide the motivation for this substantial investment are to come from the *e*A program. The capability of an EIC to collide electrons with heavy ions distinguishes the machine from any existing accelerators and makes it a unique facility. It is in these collisions where one expects new phenomena, such as saturation of the gluon densities, to be unambiguously discovered and studied. These studies will open a window into a regime where deviations from linear QCD, as probed at HERA and JLAB, become pronounced. To observe these new phenomena, it is important to verify that the proposed measurements can be conducted with both sufficient statistics and kinematic reach. An essential element of this program is a Monte-Carlo event generator that covers the broad range of physics to be investigated and goes one step further to generate events in a nuclear environment including all known and conjectured nuclear effects. Such a generator does not exist and it is the aim of this LDRD project to provide such an *e*A physics event generator. This is a crucial tool for determining requirements on the machine (energy, luminosity) and for the design of detectors at an EIC.

APPROACH:

To work on the realization of an *e*A event generator a postdoctoral fellow (Tobias Toll) was hired in summer 2010 after an extensive search. He works 100% on the LDRD project. We realized the complexity of *e*A collisions cannot be encapsulated in a single generator but that a suite of generators in a common framework will be necessary, *i.e*, the overall generator will consist of various packages that provide a common input and output format. As a first step we have focused on one of the identified key measurements at an EIC in *e*A, the study of diffractive events. Diffractive events are expected to constitute up to 30-40% of all events in an EIC and allow the determination of the gluon momentum distribution and, as the only known probe, to measure the spatial distribution of glue in a nucleus. We first focus on exclusive vector meson production (J/ψ, φ, ρ) and DVCS based on an existing dipole model (b-Sat). Once established, the program will be extended to generate also inclusive events. Here we can re-use large portions of an existing event generator. In parallel we have to simulate the breakup of the nucleus, since the fragments need to be detected to distinguish between coherent and incoherent diffraction. Once completed, we intend to move on to deep inelastic scattering (DIS) in *e*A. For DIS there is a rich set of *ep* event generators available and the most efficient path for us is to adapt an existing Monte Carlo program and extend it to generate also *e*A events. We have already worked out a method to transform the existing Monte Carlo CASCADE into an *e*A generator for DIS, a task that will be pursued in close collaboration with H. Jung, principal author of CASCADE.

TECHNICAL PROGRESS AND RESULTS:

We have completed an event generator called *Sartre* for diffractive exclusive vector meson production for *e*A collisions. The generator contains two different physics models: one that assumes a “standard” scenario (linear QCD) and one that includes the new phenomena (gluon saturation, higher twist effects) we intend to explore with an EIC. We have developed and implemented a method of calculating the cross-section for nuclear breakup to an unprecedented accuracy. The generator consists of two parts. In the first step, all extremely computing intensive tasks are performed and their results get stored in lookup tables. These massive computations could only be conducted through the intensive use of the Open Science Grid where we were able to obtain > 100k CPU hours to date. These tables are then used as input for the event generator. The resulting event generation is very fast and allows the user to generate tens of millions of events in a matter of minutes. In *ep* mode the generator reproduces existing measurements at HERA very well. This task could only be completed with intensive help, especially from T. Lappi (Jyväskylä, Finland) and R. Charity (St. Louis). Tobias Toll spent several days in Finland to develop details of the generator with Dr. Lappi.

The goal in coherent diffraction in *eA* collisions is two-fold: to get a handle on gluonic spatial structure in nuclei and its lumpiness. The key observable is the spectrum of the transverse momentum transferred from the initial nucleus to the final state, *t*, with only a vector meson in the final state, *i.e.*, events of the type e+A→ e′+A′+V. Here, and only here, can *t* be reconstructed from the kinematics of the final state particles. Events where the nucleus stays intact in the interaction are called coherent, when it breaks up they are called incoherent. It is the coherent cross-section as a function of *t* that ultimately will allow us to derive the spatial distribution of gluons in the nucleus, while the incoherent cross-section is a measure of the fluctuations/lumpiness of the gluons in the nucleus. These distributions are depicted in Fig. 1, which is generated by *Sartre 1.0* for *e*+Au→ *e*′+Au′+ρ.

One of the key signals the EIC is looking for is saturation phenomena in the large energy (low-*x*) regime. Figure 2 depicts the distribution of the center-of-mass energy of the photon-nucleus system, *W*, for *ep*, *e*Ca and *e*Au collisions in *e*+A→ *e*′+A′+ρ events generated with *Sartre*. One can see that the dramatic differences between saturation physics and the "conventional" physics scenario.

We are currently preparing two papers on the physics methods developed for *Sartre*. *Sartre* is now used in the preparation of the EIC White Paper.

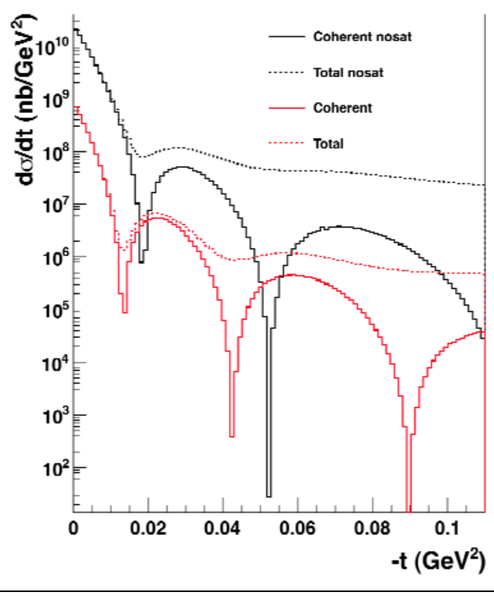

Figure 1: The *e*Au cross-section for exclusive diffractive ρ production as a function of *t*, separated into its coherent and incoherent part for saturated and unsaturated low-x gluon matter. The coherent curve represents the Fourier transformation of the spatial source (gluon) distribution.

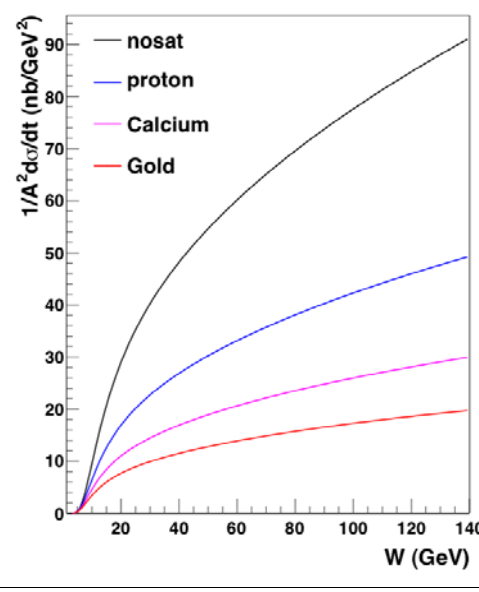

Figure 2: The cross-section as a function of *W* and divided by A^2. The saturated cross-section is quite different from the unsaturated one (nosat), which would be a clear signal for saturation when measured.

Exploring Signatures of Saturation and Universality in e+A Collisions at eRHIC

LDRD Project 10-043

Raju Venugopalan

Co-investigators: A. Dumitru, J. Jalilian-Marian, A. Stasto, T. Ullrich

PURPOSE:

A powerful motivation for an e+A collider is to study the properties of gluonic matter in nuclei at high parton density. Quantum Chromodynamics (QCD) predicts that the occupation number of gluons in nuclear wave functions saturates at a value inversely proportional to the QCD coupling. A dimensionful scale $Q_S^A(x)$ separates maximally occupied "soft" from "hard" modes that are not. This scale grows with energy and with nuclear size-for large nuclei, gluon momenta up to GeV scales are saturated. An important consequence of saturation is universality. Though naively $Q_S^2 \propto A^{1/3}$, theoretical models predict that at very high energies, the saturation scales of all nuclei approach a common value independent of the properties of the nuclei in which the gluons are confined. What are the signatures of saturation in deep inelastic scattering (DIS) off nuclei and can we extract the saturation scale uniquely from these final states? Which signatures are most sensitive to saturation? Can we anticipate precocious onset of saturation in these final states? Can they be clearly distinguished from alternative descriptions? Can one reliably extract the nuclear dependence, the impact parameter dependence, and the energy dependence of the saturation scale? By varying x and A, can we observe hints of the onset of a universal fixed point—what energy range is optimal? Reliable quantitative answers to these relevant questions are of great importance in establishing the science case for an Electron Ion Collider (EIC).

In DIS at high energies, final states can be expressed in terms of universal multi-parton "Wilson line" correlation functions. The state-of-the-art description of the energy evolution of these correlation functions is the JIMWLK functional renormalization group (RG) equation, which correspond to an infinite hierarchy of integro-differential equations. Numerical solutions of these equations are challenging [4]. Solutions to these equations correspond to determining the primary many-body content of QCD in the high energy limit. In addition to computing the properties of final states in e+A collisions, the solutions to JIMWLK RG equations are inputs in factorized expressions for multi-gluon production in proton-proton, proton-nucleus and nucleus-nucleus collisions. That is the true meaning of universality in this context, namely, the ability to use information extracted from one class of experiments to predict phenomena in other sorts of experiments.

APPROACH:

The technical advance required for quantitative studies was to solve the JIMWLK RG equations using functional Langevin techniques [1]. This goal was challenging albeit feasible as suggested by the one extant numerical computation [2]. Finally, theoretical approximations of the numerical data are essential to give insight into the underlying physics and employ results to understand data in proton-proton, proton-nucleus and nucleus-nucleus collisions. An outstanding post-doc candidate (Bjoern Schenke) was hired for this purpose and joined us in December 2010.

TECHNICAL PROGRESS AND RESULTS:

The PI and collaborators have made significant on-going progress on several fronts. Firstly, it was shown that the “ridge” correlations seen in A+A and p+p collisions are sensitive to the multi-parton correlators [3]. This was used to explain qualitatively [4] and quantitatively [5] the remarkable “CMS ridge” seen at the LHC. The effect of multiple scattering contributions to the ridge was estimated in [6]. (This included contributions by Stanislav Srednyak, a Stony Brook student supported on the LDRD.) Subsequent quantitative studies based on universality were performed for proton-proton collisions [7] and proton-nucleus collisions [8] at the LHC.

Global analyses (testing small x universality) of models explaining DIS data from HERA were applied to inclusive distributions in pp collisions at the LHC by the PI and a student Prithwish Tribedy [9]; this study further was extended to AA and pA collisions [10]. A re-analysis of new combined data from HERA, demonstrating spectacular agreement of saturation models with this data was performed by Merijn van de Klundert, a student supported on the LDRD, the PI and other collaborators [11].

With our numerical solutions, we were able to test and confirm the accuracy of a particular mean field approximation for computations of universal multi-parton correlators in high energy QCD [12]. This has proven extremely fertile ground for applying these ideas to heavy-ion collisions. In the last year, a new model, the IP-Glasma model was developed [13, 14] and shown to give excellent agreement with heavy ion data from RHIC and LHC [15] using parameters constrained from the HERA DIS data.

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Electroweak Physics with an Electron-Ion Collider

LDRD Project 10-044
William J. Marciano
Senior Members: A. Deshpande (Stony Brook University), K. Kumar (U. Mass.), W. Vogelsang (Tubingen U.)

PURPOSE:
The primary research goal of this LDRD was to elucidate the (Electroweak) physics case for polarized ep and eD scattering at the EIC, including both theory and experiment. It was divided into three parts: 1) Electroweak Structure functions, 2) Measurements of the weak mixing angle and 3) Lepton Flavor Violation.

APPROACH:
EIC offers a unique opportunity to study deep-inelastic polarized electron scattering well beyond the program at HERA, due to its anticipated higher luminosity and potential for polarizing both beams. Parity Violating Structure Functions can be measured for the first time. The weak mixing angle, arguably the most important parameter in electroweak physics, can be measured over a range of momentum transfers via the Left-Right parity violating scattering asymmetries. The lepton flavor violating transition, electron->tau, can be searched for with high sensitivity. For parts of the work, the investigators employed a postdoctoral research associate: Yingchuan Li, who was hired starting 9/1/2010 and completed his appointment in October 2012.

Issues considered included:

- What are the Machine and Detector Requirements?
- Novel Features of Parity Violation (New Structure Functions)
- Inclusion of Electroweak Radiative Corrections
- High Precision & Polarization Requirements (±0.5%?, ±0.25%?)
- Proton, D, 3He Polarization (Spin Content-Other?)
- Utility of Both Beams Polarized ?
- Higher Energy vs. Luminosity Tradeoff etc.

TECHNICAL PROGRESS AND RESULTS:

- Formulation of PV Structure Functions (Kumar & Vogelsang)
- Running of the weak mixing angle at the EIC (Li, Marciano & Kumar)
- $ep\rightarrow\tau X$ Leptoquark Sensitivity~1000×HERA (Deshpande & Kumar)

Most results were published in a report on the EIC Science case: "Gluons and the quark sea at high energies: distributions polarization, tomography edited by D. Boer et al. as a white paper that resulted from a ten week program at the University of Washington Nuclear Theory Institute.

A popular plot that resulted from this work, and was sometimes called an EIC poster, was the running of the weak mixing angle at the EIC (see Fig. 1).

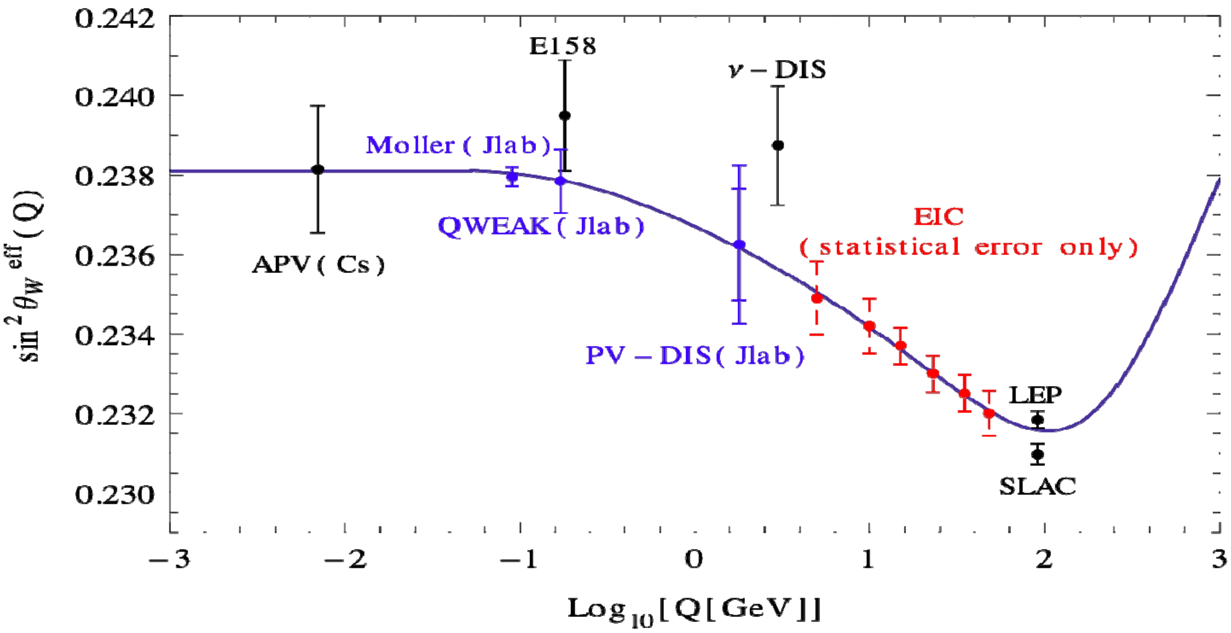


Fig. 1 A comparison of (possible) EIC weak mixing angle measurements with other existing or proposed (blue) measurements.

Measuring Dark Energy and Dark Matter using Gravitational Lensing

LDRD Project 10-045

Erin Sheldon

PURPOSE:

To measure Dark Energy and Dark Matter using Gravitational Lensing

APPROACH:

Dark Matter was discovered in 1937 but the result was ignored until the 1960s. For forty years there was slow progress in characterizing the distribution and total amount of Dark Matter. Recently the phenomenon of Gravitational Lensing, or the bending of light as it passes massive structures, has revolutionized the field. The bending of the light is directly related to the total mass, and is thus useful for measuring mass without any assumptions about the physical state of the system, or the presence of stars or gas. With lensing we can measure the location of Dark Matter and its distribution throughout the universe, limited only by the size of our astronomical survey.

In1997, Dark Energy was discovered by measuring the accelerating expansion rate of our universe. Gravitational Lensing is also sensitive to Dark Energy via the geometrical dependence inherent in all lenses: the apparent bending of light depends on the distance between the observer and the lens and source. Thus comparing the effect for sources at different recession velocities tells us about the relative distances and thus the expansion rate.

I am measuring Dark Matter and Dark Energy using gravitational lensing. My focus recently has been on measuring the distribution of Dark Matter around large clusters of galaxies, as these collections have very large mass and thus a relatively large lensing signal. My initial studies have used data from the Sloan Digital Sky Survey. I have also been working to create the Dark Energy Survey (DES), a significantly larger survey that will extend to larger distances and thus farther back in time. With measurements further back in time we can constrain Dark Energy. DES is currently in the commissioning phase. As DES winds down in 2017, I will transition to working on the Large Synoptic Survey Telescope (LSST).

My work is to measure the fundamental observable of lensing: the gravitational shear. I then interpret this shear in terms of the distribution of Dark Matter and the properties of Dark Energy.

Measurement of gravitational shear is not a solved problem, at least at the level needed for DES and LSST. The shear changes the shape of galaxies, inducing an ellipticity. Galaxies themselves are inherently elliptical, but with random orientations. Lensing induces correlations in the orientations. However, the atmosphere and the optics can also induce correlations, known as the Point Spread Function (PSF), and these effects must be corrected, or calibrated. In the presence of noise, these effects are difficult to remove.

I am developing a technique to correct for the effects of the PSF in the high-noise regime. I use a mixture of Gaussian components to represent the PSF effect and the galaxy. I apply Bayesian techniques, in particular a prior on the ellipticities of galaxies, to mitigate the effects of noise.

I am also working on the interpretation of shear. One component of this problem is to measure the correlations in the ellipticities of galaxies; this is a solved problem.

Another, more difficult component of the interpretation is the distances to the background sources. These galaxies are too faint to measure recession velocities via spectroscopic techniques. We must instead infer their distances statistically based on crude color information (placing filters over the camera). This method is known as photometric redshifts. Collaborators and I have developed a new technique to recover the distribution of distances given the multi-dimensional distribution of colors.

The final component interpreting the shear is to generate the predicted signal. With collaborators, I am developing the models appropriate to infer the distribution of Dark Matter and Dark Energy in the universe.

TECHNICAL PROGRESS AND RESULTS:

In previous years, progress was made developing a new software pipeline for analyzing astronomical images to measure gravitational shear effects, and correct for the point spread function. The framework developed is useful for all techniques.

In the last year great progress was made. I developed a new technique for measuring shear, mentioned in the approach section above. This technique, using Gaussian mixtures and Bayesian formalism, is more accurate than the software developed in previous years. This work is nearly complete and will be published shortly. In the coming months, I will apply this technique to images from the Sloan Digital Sky Survey and the new Dark Energy Survey.

Significant progress was also made on the "photometric redshift" technique mentioned in the approach section (the statistical measurement of distances to galaxies). Extending our previous work, we generated the largest ever catalog of photometric redshifts, and demonstrated they are the most accurate such measurements to date. This work was published in Sheldon et al. 2012 with close collaborator Carlos Cunha.

Collaborators and I published two papers interpreting the gravitational lensing effect in terms of Dark Matter and Dark Energy. The first involved comparing the Dark Matter distribution in clusters of galaxies to the distribution of light (Tinker et al. 2012). The second involved using the large-scale correlations of Dark Matter with cluster locations (Zu et al. 2012).

Postdoc Zhaoming Ma completed a very important work for calibrating gravitational lensing measurements. Given measurements of the ellipticities of stars (the "points" in the Point Spread Function), one must interpolate that information to the location of galaxies. There are not enough stars in an image to do this accurately. Zhoaming completed a code to find principal components of the PSF using all images of a survey, which means many fewer stars are needed per image to perform the interpolation. His technique is sufficient to meet the needs for the Dark Energy Survey and the future LSST.

Cloud and Precipitation 4D Radar Science

LDRD Project 11-001

Scott Giangrande

PURPOSE:

Deep convective clouds (DCCs) play a critical role in Earth's climate system. Understanding the properties of these clouds and simulating their impact is a major challenge for current global climate models (GCMs) and cloud resolving models (CRMs). DCCs are particularly difficult to adequately observe and model since their dynamical, microphysical and radiative feedbacks act over a wide range of scales. This LDRD capitalizes on a new cloud observing facility strategically positioned in an environment favorable for DCC development. This unique testbed provides an opportunity to overhaul traditional cloud observations and assess the environmental controls that influence the lifecycle and morphology of DCCs. Our objective is to innovate novel observations of convective cloud properties and atmospheric controlling factors to enhance our understanding of these cloud systems towards significantly improving CRM/GCM performance.

APPROACH:

A. Background and Scope: New Multi-scale Observing Facility Capability: The DOE Atmospheric Radiation Measurement (ARM) Climate Research Facility (ACRF) located in central Oklahoma underwent a major upgrade towards providing unprecedented observations of DCCs. Of immediate interest for characterizing DCC evolution is the suite of scanning cloud and weather radar, each tasked to operate over progressively larger and overlapping domains. These systems include first-ever scanning cloud radar (millimeter wavelength) to map initiating clouds, as well as large-umbrella weather radar (centimeter wavelength) for bulk quantification of deeper precipitating storms. The radars allow detailed microphysical insights with sensitivity to capture clouds as they form. Here, the opportunity exists to assume leadership in multi-sensor synergistic approaches to climate-cloud observations for GCM/CRM evaluation. The traditional DOE ARM model relies on individual remote-sensing platforms, but this is not sufficient since individual radar systems only capture a brief snapshot of DCC cloud life cycle. Further, DOE ARM lacks expertise in observing deep precipitation processes. Exploiting multiple radar synergies for cloud and precipitation lifecycle study has never been attempted, but has the potential to yield far more meaningful advances in our understanding of DCCs for improving model parameterizations.

B. Methodology: Deep Convective Storm Tracking and Characterization:

Scanning radar systems provide an opportunity to map cloud evolution since they can observe cloud particles at spatial and temporal scales sufficient for continuous monitoring. An individual radar platform is only sensitive to specific stages of cloud development as a consequence of the radar wavelength and other hardware limitations. We propose to observe the possible DCC lifecycle as follows. (1) Capture 4D (space + time) cloud evolution by exploiting the synergy of complementary, overlapping radar platforms. This is our best opportunity for DCC monitoring, but for the observations of initiating clouds in particular, adaptive scanning of cloud systems is unique, exploratory and therefore risky since our observational capabilities may not be sufficient. The effort further requires (2) detailed tracking of initiating cloud elements using a variety of novel approaches to assess the best techniques to observe representative cloud properties. This must be performed in coordination with (3) identification of the specific cloud properties that best translate across the overlapping radar domains (e.g., radar reflectivity factor, cloud base/depths). Efforts in (2) and (3) benefit from additional support from collaboration with McGill University radar and cloud experts on an LDRD subcontract. Finally, individual case studies must (4) package the 4D observation quantities in a manner easily accessible for GCM/CRM model improvement; e.g., linking with the atmospheric conditions that forced these clouds.

TECHNICAL PROGRESS AND RESULTS:

Previous Year (2011) Progress: In year one (Y1), the LDRD was critical towards conducting a successful field campaign allowing application of first-ever climate monitoring systems to characterize cloud lifecycle that has direct implications for our ability to predict possible climate change. Y1-based accomplishments include direct demonstration of networked radar facilities for unique DCC characterization through 12 conference presentation/poster efforts. The subcontract partnership between the PI and the McGill graduate student has identified 'golden' events from the campaign period and preliminary analysis suggests the data collected will be sufficient to address cloud initiation and early stage cloud/precipitation tracking goals of the LDRD. End of Y1 subcontract graduate student activities included working towards public demonstration of unique tracking capabilities of individual cloud elements and their evolution from ground-based radar systems and collocated observations for a particular event of interest (May 25th, 2011).

Current Year (2012) Progress: In year two, the PI and graduate student merged the radar dataset and forcing record for analysis and cloud modeling connectivity. We engaged in a collaboration with Kansas University cloud modeling experts to begin detailed large-eddy simulation (LES) model comparisons for the May 25th, 2011 shallow cumulus event. Model-observation LDRD partnering will continue into 2013 under the McGill student's leadership (LDRD subcontract). 2013 milestones under this partnership include associated publications on cloud radar insights to LES cloud modeling. Encouraging initial results from cloud tracking methods also provide a solid justification for resubmission of a follow-on proposal on shallow cumulus cloud lifecycle.

Initial journal publications from 2011 efforts towards deep convective radar processing and intensity observations were accepted for release in 2013. A student-led publication on the LDRD cloud tracking algorithm and its associated results is in preparation for 2013 submission. Overview manuscripts describing the 2011 campaign and the new DOE capability for radar precipitation products and insights are also in preparation.

A Novel Approach to Parameterize Sub-Grid Processes in Climate Models

LDRD Project 11-002

Dong Huang

PURPOSE:

The purpose of this project is to develop a novel statistical approach that allows for consistent treatment of sub-grid processes in Global Climate Models (GCMs). The new approach will offer a way to easily transfer knowledge learned from surface-based or satellite cloud observations into climate models. This project will also facilitate collaborations between the BNL atmospheric research group and wider climate modeling groups outside BNL.

APPROACH:

Physical processes acting at spatial and temporal scales that are too small to resolve by the numerical grids of GCMs are presented in climate models using parameterizations. A parameterization is a statistical description of the effects of the subgrid processes and interactions in terms of the resolved-scale state. Therefore, parameterizations are statistical in nature. Conventional parameterizations used in current GCMs (e.g., cloud feedback and aerosol-cloud interaction) are developed empirically and sometimes are inconsistent with each other.

Using more rigorous statistical methods, we have developed a new framework that utilizes explicit subgrid variability, i.e., subgrid Probability Distribution Functions (PDFs), to formulate parameterizations.

As illustrated in Figure 1, two different approaches have been investigated to explicitly account for subgrid variability: a direct approach and a Monte Carlo approach. The direct approach is to analytically integrate the relevant subgrid processes over the subgrid cloud PDF. For mathematically-simple processes (e.g., autoconversion, collection, and evaporation), this direct approach is attractive because the addition of computational cost is negligible. In the Monte Carlo approach, a statistical realization of cloud field (subcolumns) will be generated using a statistical cloud generator under the guidance of the subgrid PDF. Other subroutines then can be directly applied to the subcolumns and the grid-averaged quantities can be obtained by cleverly sampling the subcolumns. The Monte Carlo approach could be the only option for some complex processes for which analytical integration is difficult or impossible to perform.

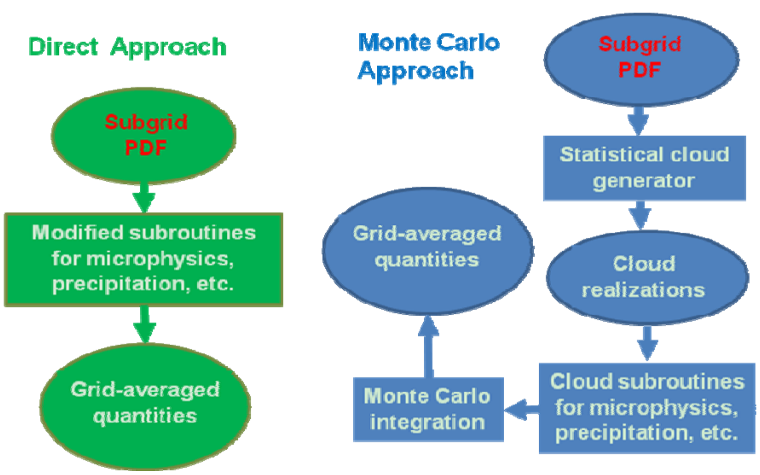


Figure 1: Two approaches for explicitly accounting for subgrid cloud variability.

TECHNICAL PROGRESS AND RESULTS:

This project officially started in October 2010. There are two researchers working on this project, Dr. Dong Huang (the PI) and Dr. Michael Galletti (joined us as a research associate in August 2011). Dr Galletti is fully supported by this project.

In FY2011, we performed in depth analysis of the decade-long cloud dataset to examine subgrid-scale cloud variability and structural function. It was found that PDFs of cloud water content can be accurately described by Gamma functions at relative large scales (spatial scale > 100 km or temporal scale > 3 hours). In FY2012, we developed and coded a statistical (or stochastic) radiative transfer parameterization scheme that directly uses a subgrid cloud PDF and cloud spatial correlation function. Through the use of statistical information of subgrid-scale clouds, the grid-mean radiation parameters can be accurately computed (Figure 2). The statistical approach does not require knowledge about the exact 3D spatial distribution of cloud properties and it instead uses a statistical distribution function of the clouds. It is important to point out that the statistical parameterization approach developed during the project is not only applicable to radiation transfer problems in the atmosphere but also applicable to many other disciplines such as biological imaging and neutron transport.

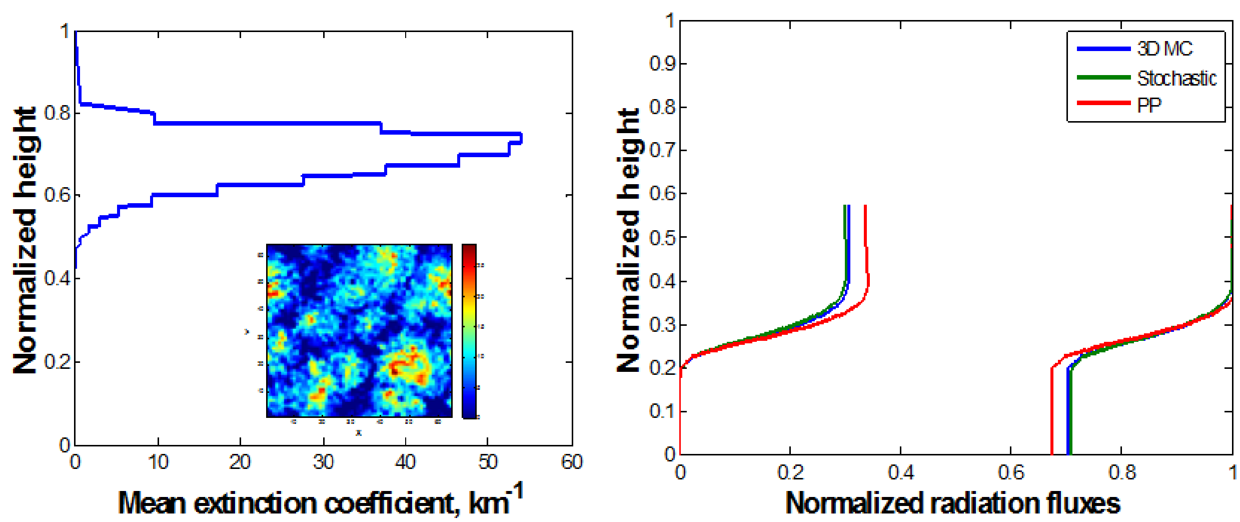


Figure 2: Demonstration of the statistical radiative transfer parameterization. The left panel shows the cloud field and the vertical profile of mean cloud extinction coefficient. The right panel shows the computed mean radiative fluxes using three different approaches: 3D MC (Monte Carlo approach using detailed 3D clouds), stochastic (the statistical approached developed by us), PP (1D approach ignoring subgrid cloud variation).

In FY 2013, we will focus on testing the statistical radiative transfer method and optimization of the code. The FASTER Testbed will be used extensively during the proposed parameterization evaluation and improvement research. The new parameterizations developed here will be integrated into the FASTER Testbed to allow for broader tests by other researchers. Parameterization tests in a global context thus will also be performed in collaboration with the FASTER team.

Deciphering the Molecular Mechanisms of Lignin Precursor Transportation

LDRD Project 11-007

Chang-Jun Liu

PURPOSE:

Lignin is the second most abundant biopolymer after cellulose in plant secondary cell walls. While important for plant viability, its presence in cell walls contributes to the wall's recalcitrance and formidably impedes the conversion of cellulosic biomass to biofuels. Better understanding on cell wall lignification will facilitate the manipulation of lignin content and composition, thus to better tailor lignocellulosic biomass structural property and create new types of bioenergy crops for both sustainable biomass production and effective cellulosic biomass conversion. Lignin is derived primarily from the condensation of three monomeric precursors. Previous studies noted that lignin is differentially deposited in particular tissues or cells, implying a tightly regulated and selective export and deposition of the precursors into cell walls by an active transport process, in which some membrane transporters may actively support both the intracellular sequestration, and the export of monolignols across plasma membrane for polymerization. However, direct biochemical and molecular evidence is essentially lacking.

The goals of this project are to biochemically evaluate the mechanisms underlying the intra- and inter-cellular translocation of lignin precursors in plants; and to genetically screen and preliminarily assess the particular membrane transporters potentially involved in cell wall lignification. Success in understanding the lignin precursor transport process may lead to a rational solution for the temporal- and spatial-control of the deposition of lignin in the cell wall, therefore, producing desired lignocellulosic biomass for agricultural and bioenergy industrial applications.

APPROACH:

We are employing biochemical-reverse genetics approaches including gene knock-down/out, RNAi mediated gene suppression and over-expression, and the comprehensive phenotyping and chemical analysis of cell-wall composition to identify the particular membrane transporters functioning in cell wall lignification.

TECHNICAL PROGRESS AND RESULTS:

In FY 2012, we primarily focused on the characterization of a small set of selected membrane transporters (ABC and META type transporter proteins).

- We systematically examined the physiological phenotypes of the screened homozygous T-DNA insertion mutant lines and the created gene suppression plants of individual transporters. Alteration of growth and development of their different tissues/organs was recorded.
- Soluble metabolites and cell wall component and compositions of the mutant and gene suppression plants were comprehensively analyzed by histochemistry, and/or liquid/gas chromatography mass spectrometry.
- Promoter regions of a few transporter genes were isolated and the tissue specific and spatial gene expression patterns of individual transporters were determined by Promoter::GUS assay.
- Full length cDNAs/genes of individual transporters were isolated, which were used for heterologous protein expression in either a yeast or insect cell system and for ectopic

overexpression *in planta*.

- The transporter-green fluorescent fusion proteins were constructed and their subcellular localization in plant cells was examined by transient or stable expression.
- In order to explore the potential biochemical functions of transporter proteins, several expression systems, including yeast, tobacco BY2, and insect cells as well as protoplasts derived from overexpression plants were developed and tested.

Based on these studies, particular transporters that are potentially involved in translocation of phenolics, and hormones that affect vascular cell differentiation and lignification were preliminary identified.

Touchless Micro-Crystallography

LDRD Project 11-008

Alexei Soares, Allen Orville, and Marc Allaire

PURPOSE:

The LDRD explores novel methods for preparing, improving, and exploiting protein crystals using acoustic methods. Major initiatives for preparing protein crystals include micro crystallization, crystallization promoting additives, and two-component co-crystallization. Major initiatives for improving protein crystals include two-component post-crystallization soaking experiments, cryo search, and crystal seeding. Major initiatives for exploiting protein crystals include various novel crystal injection systems.

APPROACH:

Our most important collaboration has been with LabCyte, a company that manufactures and markets acoustic technologies. We have also collaborated with MiteGen, a company that designs solutions for crystallization and crystal mounting. In addition, we also collaborate with Plasma Science Innovation (PSI) centers to obtain protein samples (mostly Steven Almo's group at Albert Einstein College of Medicine).

TECHNICAL PROGRESS AND RESULTS:

Initial proof of concept (i.e. that crystals can be successfully manipulated with sound waves, without damage) was demonstrated and published [A. Soares et al., Biochemistry 50(21): 4399-4401 (2011)]. A commercial Echo® 550 liquid handler was acquired in September 2012. Individual milestones toward each of the objectives of this LDRD are as follows:

1) Crystallization: Two novel protein crystallization conditions were identified using the Echo® 550.

2) Crystal improvement: Two component sample preparation is now routine. We prepared and cryogenically preserved 192 two-component specimens (crystal + fragment library) in under two hours. Data acquisition from these specimens required 8 days of beam time at GM/CA beam line (Advanced Photon Source, Argonne National Laboratory) and X25 beam line (NSLS). Our rates of specimen preparation are high enough to fully engage beam lines with the projected intensity of NSLS-II.

3) Crystal exploitation: We have constructed and tested a custom built in-house crystal injector for installation at the SLAC National Accelerator Laboratory Linac Coherent Light Source (LCLS). We have received an invitation from the LCLS Director to use equipment (no-beam) time in early 2013 to commission our instrument. We have also received a 5-day experimental beam-time assignment in June 2013.

Funding: We submitted an RO1 research proposal to the National Institutes of Health which was not funded. Our concepts are a key component of the XO2 pre-proposal for a P41 Center at NSLS-II.

Multiscale Complexity of Energy and Material Use: Integrated Assessment of Technology and Policy Alternatives

LDRD Project 11-012

J.- K. Choi & Paul Friley

PURPOSE:

The specific research goals of the proposed work included theoretical and applied aspects as follows: 1) Develop a framework, which synthesizes environmental life cycle assessment with existing energy economic modeling tools for analyzing energy systems across multiple temporal and spatial scales and provide valuable insights into their complex interrelationship with other systems, 2) Apply the framework to evaluate existing and proposed economic/energy policies for reductions in the environmental impacts of energy technologies, particularly for the transition to advanced renewable energy technologies and intermediate policies for a smooth transition between policy regimes. This research topic is intriguing not only because of its scientific and environmental relevance, but also due to the challenges it presents to engineers, economists and policymakers. This research will meet the LDRD Program goals and the DOE mission by employing the multi-disciplinary research approaches to develop technology and policy analysis tools to underpin the national climate change policy, as outlined in BNL's strategic plan for FY09 – FY18.

APPROACH:

Many different energy economy modeling tools are available but most methods for technology assessment and policy analysis tend to focus on the macroeconomic scale level. Methods for transferring information and effect of decisions across multiple scales are inadequate. Such methods are essential for evaluating the effect of changes or policies implemented at coarser scales on activities at finer industry scales or their value chains. Such techniques are also essential for determining the effect of engineering decisions and new technologies introduced at finer scales on coarser scales of the supply chain and economy. A combination of both Market Allocation (MARKAL) and Life Cycle Assessment (LCA) is promising to incorporate the strength of both methods. There are some studies to feed economic and environmental parameters into the MARKAL model that allow for the consideration of additional aspects such as restricted resource availability or learning curves. However, tools for analyzing the dynamic impact of certain policy to the life cycle environmental impact in a product system level are scarce. This research proposed a general framework for performing a multiscale futuristic LCA (MF-LCA) of a product system by combining these two tools. New energy standards such as ISO 50001 require industries to commit to the efficient energy use on their production process and supply chain management while meeting their emission abatement goal. In addition to these voluntary actions, different energy policies, such as carbon taxes and cap-and-trade, affect the supply and demand of energy commodities both directly and indirectly. Both policy makers and industrial managers need to understand the impact of energy policy to the environmental profile of industrial processes for preparing effective energy policies and strategic corporate management decisions, respectively.

TECHNICAL PROGRESS AND RESULTS:

This project significantly enhanced techniques for evaluating the life cycle economic, environmental, technological and social aspects of energy systems under different policy scenarios. The framework enables a wide range of applications for integrated assessment of multiscale complex problems. The framework also facilitates whole systems analysis for national/state level policy by complementing well-established tools or providing alternative technology solutions. In addition, it can help various industries improve their strategic business decision making on production and service activities through the proposed integrated optimization process.

In FY 12, the research focus was on analyzing dynamic change of environmental life cycle impact of a production system under a range of potential climate policies. After the static Life Cycle Inventory (LCI) for a system was formed, average electricity used for each product life cycle stage in the static LCI was disaggregated with respect to the percentage electricity generation mix information gathered from MARKAL for each time period and policy. Then the change in emission intensities for fossil fuel based electricity generation over the time period was considered to create a dynamic LCI database for a product life cycle. An impact assessment method, Tools for the Reduction and Assessment of Chemical and other Environmental Impact (TRACI), was used for analyzing the dynamic change of the various environmental impacts on the production processes. From the MARKAL side, various carbon mitigation policies are considered in the U.S. Multi-region MARKAL (US MRM). The main source of technology assumptions for the US MRM is the Energy Information Administration (EIA). Much of the relevant information is published annually as part of the Annual Energy Outlook (AEO) and the associated National Energy Modeling System (NEMS) documentation.

The dynamic life-cycle inventory database developed in the prior year was utilized to assess the changes in the future life-cycle environmental impact of a current product/process system for producing crystalline silicon photovoltaic panels under four different emissions policy scenarios. The results of this case study were published in the journal Renewable and Sustainable Energy Reviews in September 2012. The results of this research were also presented at the 15th Energy Utility Environment Conference and the International Symposium on Sustainable Systems and Technology. Activity on this LDRD concluded August 16.

Publications

1. J.- K. Choi , P. Friley, and T. Alfstad, “Implications of energy policy on a product system’s dynamic life-cycle environmental impact: Survey and model”, *Renewable and Sustainable Energy Reviews, 16 (7), pp 4744-4752, 2012.*

Conference Proceedings

2. J.- K. Choi, and P. Friley, “Dynamic LCA of Energy Technologies ” *International Symposium on Sustainable Systems and Technology,* Boston, MA, May 16, 2012.

3. J.- K. Choi, and P. Friley “The Implication of the Energy Policy to the Dynamic Life Cycle Environmental Impact of a Product System” *15th Energy, Utility, Environment Conference,* Phoenix, AZ, Jan. 31, 2012.

Indium Iodide (InI) – A Potential Next-Generation Room-Temperature Radiation Detector

LDRD Project 11-016

Anwar Hossain

PURPOSE:

There is widespread demand for high-performance, compact radiation detectors in many areas, including homeland security, medical imaging, and astrophysics. Cadmium Zinc Telluride (CZT) detectors are currently the leading candidate in these applications. However, their deployment has been limited by the dearth of high quality, large-volume single crystals due to material defects, primarily generated during crystal growth. A near-term remedy of such issues remains challenging, since the technical issues in growing crystals seemingly cannot be overcome easily. For better balance in our detector program, we opted to search for a suitable alternative detector material. While several materials are in the pipeline, all still are far from offering an alternative to CZT. Furthermore, current semiconductor detector materials contain toxic elements which might be deemed as health- and environmental- issues in the future. In view of the features, we proposed Indium Iodide (InI), a binary compound semiconductor, which may be a promising candidate for the next-generation, room-temperature radiation detectors.

APPROACH:

Indium Iodide possesses the required properties for an excellent radiation detector and offers several potential advantages over other materials for room-temperature radiation detection and imaging. It has a relatively low melting point (381ºC) and does not exhibit a solid-solid phase transition between its melting point and room temperature. Therefore, we can grow flawless large single crystals readily via simple melt-based processes, like the Bridgman technique. We have well-established crystal growth and characterization facilities and supporting scientists at BNL to execute all the steps from crystal growth to device testing. Our goal is to complete comprehensive feasibility studies of InI as a next-generation room-temperature semiconductor detector.

TECHNICAL PROGRESS AND RESULTS:

We began the process of purchasing source materials immediately after this project began in October 2010. We received the source materials around February 2011. The initial purity of the InI source material was 5N grade, and in order to improve the material purity we conducted zone refining with 50 passes at 405 °C and at 20 mm/hour speed in a carbon-coated quartz ampoule. Afterward, we used a floating zone method to grow the crystals. The growth temperature was 395 °C with a temperature gradient 25 °C/cm, and the growth rate was 2.0 mm/hour.

We anticipated problems during our first approach as one of the motors stopped functioning after 15 passes of the zone-refining process, which yielded a defective ingot. We optimized the system after replacing the motor and grew another ingot. We characterized its material properties, fabricated the detectors, and tested them as X- and gamma-ray radiation detectors. The purification system, crystal growth furnace and as-grown InI crystal are shown in Figure 1.

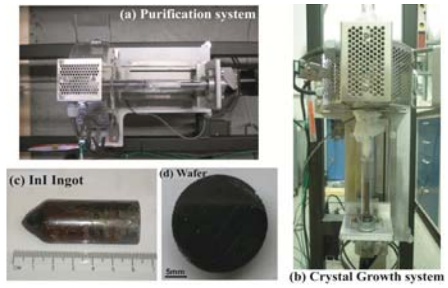


Figure 1.(a,b) Material purification and crystal growth system; (c, d) As-grown ingot and a wafer of InI crystal.

The ingot was sliced and cut into the desired size, and processed for characterization of its bulk properties. The band-gap was measured using the Fourier Transform Infra-Red (FTIR) method, and a value of 1.96 eV was obtained. We investigated and captured infra-red (IR) transmission images of polished wafers, which displayed that the entire ingot was likely to be single crystal. There are some voids generated in the ingot during crystal growth; those are most likely due to an improper cooling rate. We should be able to resolve this problem in our next growth process. We also analyzed the material uniformity using Scanning Electron Microscopy integrated with an Energy Dispersive X-ray Spectroscopy system. The composition of elements was found to be fairly uniform along the radial direction of the wafer. We processed some selected crystals and attached metal contacts for electrical measurement and device testing. We measured the leakage current against bias voltage and calculated the resistivity of the crystal (~10^{11} Ω-cm). We tested them as radiation detectors using an Am-241 source and obtained reasonably good response. However, the detector showed a polarization effect and the peak disappeared. More investigation is needed to understand and resolve the polarization.

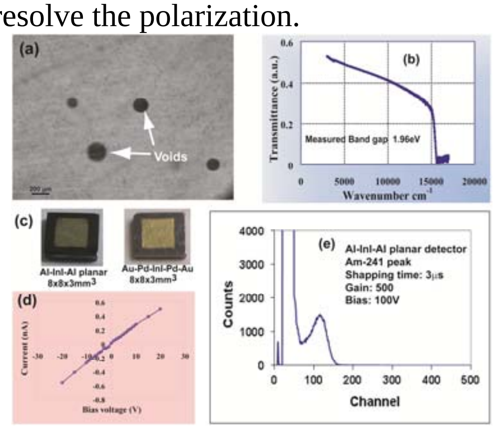


Fig. 2. (a) IR transmission image of InI wafer. Voids were found in the wafers; (b)Band gap was measured by the FTIR method; (c)Images of InI planar detectors; (d) Current-voltage curve; (e) Am-241gamma response of an InI planar detector.

High-resistivity, large-volume single crystals with fewer defects were successfully grown. Our research indicates that it is a promising candidate material for room-temperature and gamma-ray detectors in the field of homeland security, industrial/medical imaging and high energy research.

Milestones:

Year 1: (1) Optimize material purification and crystal growth process; and
(2) Material characterization, device fabrication, and testing.

Year 2: (1) Crystal growth after modifying the parameters from acquired feedback; and
(2) Material characterization, device fabrication and testing.
(3) Apply for DOE/other funding based on these acquired data.

Visualization Support Infrastructure for Global Climate Modeling with a Focus on the BNL FASTER Project

LDRD Project 11-017

Michael McGuigan (BNL, Computational Science Center)
Klaus Mueller (Stony Brook University, Computer Science Department

PURPOSE:

The objective of this project is to develop an interactive visual analytics system that can aid atmospheric scientists in the analytics and refinement of global climate models. We have collaborated closely with the BNL FASTER team led by Yangang Liu to implement, test, and evaluate the developed system.

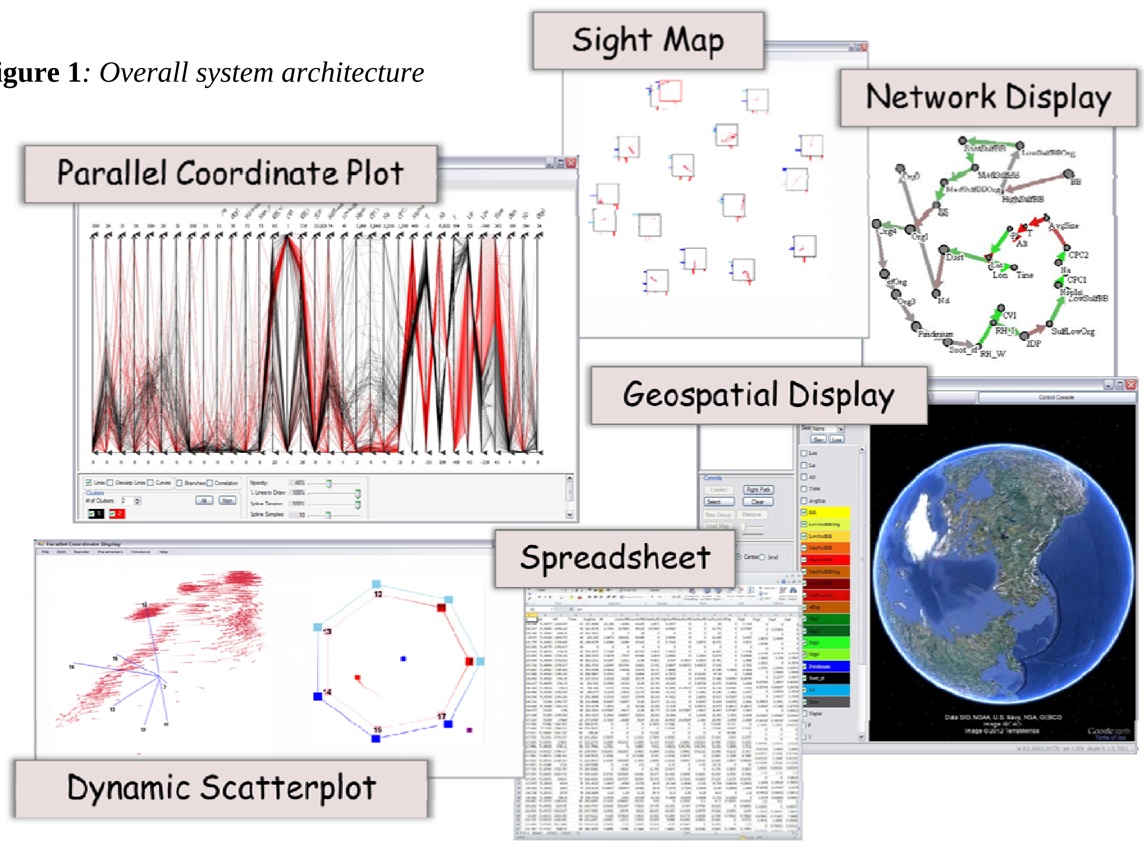
APPROACH:

The FASTER climate data has a wide range of time-variant variables, including but not limited to cloud macrophysics, such as cloud fraction, base and top height, liquid/ice water path, and precipitation, as well as aerosol properties and radiation fluxes. Devising a visualization suite tailored to the data configuration of the FASTER project was the aim of this 2-year project. Our approach was to extend and adapt a suite of multivariate visualization tools we have already developed and link them with an interactive geo-spatial display based on Google Earth augmented to provide multivariate visualization capabilities.

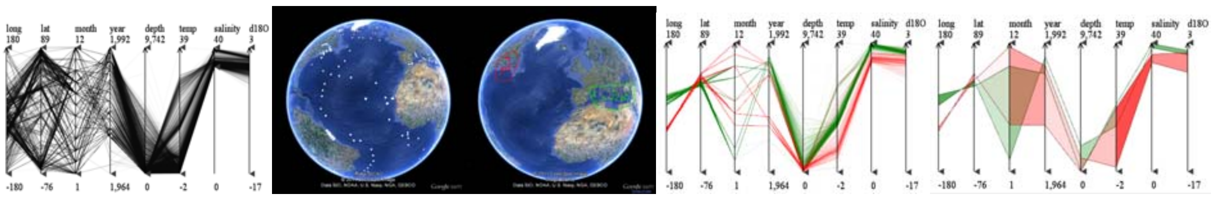
TECHNICAL PROGRESS AND RESULTS:

Figure 1 illustrates the various components of our developed system. The *parallel coordinate plot* shows the raw multivariate data – each vertical axis represents one attribute and each data point gives

Figure 1: *Overall system architecture*



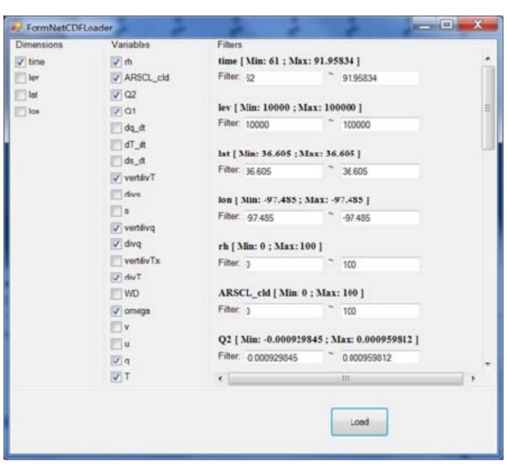
rise to a piecewise linear line going across the axes. The *dynamic scatterplot* is a projection of the multivariate data into an arbitrary vector basis controlled by the polygonal touchpad interface shown on the right – each vertex is due to one chosen data attribute, here 7. The *sight map* can be used to save interesting projections and arrange them in terms of their projection vector similarity. The *network display* arranges the data dimensions in terms of their correlation – nodes of closely correlated attributes are located nearby – and users can define a path across this dimension landscape to specify and axis order in the parallel coordinate plot. The *geospatial display* allows users to visualize and select geo-referenced data within a Google Earth plug-in – the data marked there are then highlighted in different colors in the parallel coordinate and the dynamic scatterplot display where they can be further manipulated. Finally, the *spreadsheet* enables users to perform mathematical operations on the data and so create new attributes that can be visualized in the various linked display. Fig. 2 shows the system in action, using the Global Seawater Oxygen-18 dataset.



(a) (b) (c) (d) (e)

Figure 2*: Dual-domain analytics. (a) The analyst first uses the PCP (parallel coordinate plot) brushing handles to select the normal ocean data points (salinity from 32-40). (b) The GE (Google Earth) display responds by showing only these remaining data points. (c) Next the analyst uses mouse clicks to outline some interesting regions in GE (Mediterranean shown in green and Gulf of St Lawrence shown in red). (d) The points inside the selection polygon appear highlighted in the PCP. (e) Correlation-enhanced illustrative PCP display.*

In year 2 we have focused on making the program accessible to the FASTER scientists. First, we have written a detailed and richly illustrated manual (26 pages), which the scientists requested. The delivery of the manual and software will be soon. Second, we have added support for NetCFD files, which is the format the FASTER scientists prominently use. We developed a graphical user interface (GUI) (see Fig. 3), which allows them to manage the many variables and also to subsample massive datasets to make them manageable for visual interaction. As an added feature for convenient interaction, the program remembers these settings such that they do not have to be specified again when the dataset is visualized next time. The final feature – support for time-lag correlation – is still under development. This is an interesting research topic and we will use the correlation network display to visualize the temporal interaction among variables.



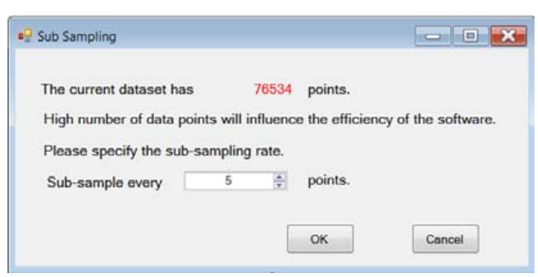


Figure 3: *GUI for NetCFD files. Scientists can use the above GUI to select variables, and the below GUI allows them to specify a subsampling rate to manage massive datasets.*

Single Crystal Growth of Novel Energy Materials by High Pressure Method

LDRD Project 11-020
Genda Gu

PURPOSE:

Our goal is to explore single crystal growth of advanced energy materials. In particular, we will address the problem of growing crystals with highly volatile components that cannot be grown at ambient pressure. Our approach is to develop a new technique to grow various single crystals involving our new and unique use of high-pressure hot isostatic press furnace.

APPROACH:

By using a super-high pressure furnace, we will explore the growth of the single crystals of various new advanced energy materials, which can not be grown at ambient pressure by traditional crystal growth methods. A new high pressure hot-isostatic press furnace, with capability of gas furnace, which will have a gas pressures (a gas mixture of 20% oxygen or nitrogen—80% Ar) up to 7000 bars and temperatures up to 1200°C initially (with the potential for 2000°C) and a working volume of 1.5 inch diameter by 6 inch high, will be installed in our group in Jan. 2011. The furnace is the first of its kind in the world, offering us new capabilities to explore various new single crystals, which cannot be grown in other groups in the world. We specifically address the newly discovered highly volatile energy materials that cannot be grown at ambient pressure, an area in which there is great potential for discoveries as well as for improvement in techniques and capabilities. For example, all rechargeable lithium electrode materials, such as $LiMn_2O_4$ (cathode materials), $Li_4Ti_5O_{12}$ (anode materials) can never be grown into mm-size single crystals due to the highly volatility of Li_2O high volatile nature at the melting point. In order to provide the major breakthroughs needed to address important fundamental science and technology questions, the large single crystals are indispensable for us to study the fundamental issues on the complex chemical and physical phenomena in the electrode materials. There are three types of energy materials we will try to explore: 1. lithium battery electrode materials; 2. new nitride materials for solid state lighting; 3. new oxide and non-oxide superconducting materials. If the new single crystals of advanced energy materials are grown, it will put BNL to the forefront of the energy materials research that will bring future research funding from DOE and industries.

TECHNICAL PROGRESS AND RESULTS:

For FY 2012, we have hired a new post-doctoral fellow, Zhijun Xu, to prepare the high-pressure work. We have installed the high-pressure furnace from AIP in Chemical Building in our laboratory (The HIP furnace is shown in Figure 1). Our 1,000,000 psi hot isostatic pressure furnace is the best furnace in the world.

Fig. 1, the picture of 1,000,000 psi hot isotatic pressure furnace installed in Chemical Building.

We have annealed the various new single crystals by using the new hot isostatic pressure furnace, such as double layer superconductor single crystals $La_2CaCu_2O_6$ and $La_2(Sr_{1-x}Ca_x)Cu_2O_6$. It is the first double layer La system oxide superconductor with T_c=55K in the world.

Protein Microcrystal Dynamics by Coherent X-ray Scattering

LDRD Project 11-025

Andrei Fluerasu

PURPOSE:

The intimate relationship between the structure of biomolecules and their biological function has been established for a long time and has lead to the outstanding development of fields of research such as protein crystallography (PX). However, function requires *motion*. The LDRD project focuses on developing an experimental pathway and a general method for measuring the time scales associated with molecular motion in biomolecules using coherent X-ray diffraction. With the advent of high brightness synchrotron sources such as the NSLS-II, this method will be particularly useful for measuring relatively slow (e.g. ~1 ms) collective dynamics in protein systems. The time scales associated with collective molecular motions will be measured using diffuse X-ray scattering and *X-ray Speckle Visibility Spectroscopy* (XSVS).

This method will be complementing Neutron Spin Echo (NSE) studies of fast molecular dynamics and Nuclear Magnetic Resonance (NMR) measurements of individual bond vector motion in small molecules.

APPROACH:

At the current stage of the project the intensities available as 3rd generation synchrotron sources such as the APS allow measurements of diffuse coherent X-ray scattering patterns (a.k.a. *speckle* patterns) only over relatively long integration times (e.g. on the order of ~1 s). When the samples are held at room temperature, the beam-induced damage does not allow recording more than just a few frames from a single location in the sample. The main idea that we are trying to pursue is to repeat the same (or nominally the same) experiment at different locations across the sample to enhance the statistics of the measured signals. It should also be noted that in the medium term with coherent intensities that will be 100x higher at the CHX instrument at NSLS-II, the same measurement will be performed in ~1 ms instead of 1 s. This will allow measuring a number of slow motions of the protein system.

The first goal of our experiments was to measure static disorder in protein crystals resulting from “frozen” molecular motions and/or static microstructural defects. Several different samples which were held either at room temperature inside of thin and sealed quartz capillaries, or held by standard PX sample loops after being flash-frozen in liquid nitrogen. In order to allow precisely positioning at different locations the beam and scanning the entire crystalline sample, an on-axis optical microscope was built.

TECHNICAL PROGRESS AND RESULTS:

The first important result of this research program came from concanavalinA (conA) which is a carbohydrate-binding protein originally extracted from jack-bean. Crystals of conA were grown using a counterdiffusive ion method directly inside thin quartz capillaries which are well adapted for coherent X-ray scattering. Our experiments proved that these samples are high quality crystals with a very low mosaicity which can produce, nevertheless, static speckles in the diffuse scattering evidencing some form of disorder correlated over relatively large distances (several unit cells). The experiments are severely photon limited (Figure 1) but prove nevertheless that with the intensities that will become available at NSLS-II, we may be able to measure time constant associated with collective (i.e. correlated over several unit cells) motions on the order of 1 ms.

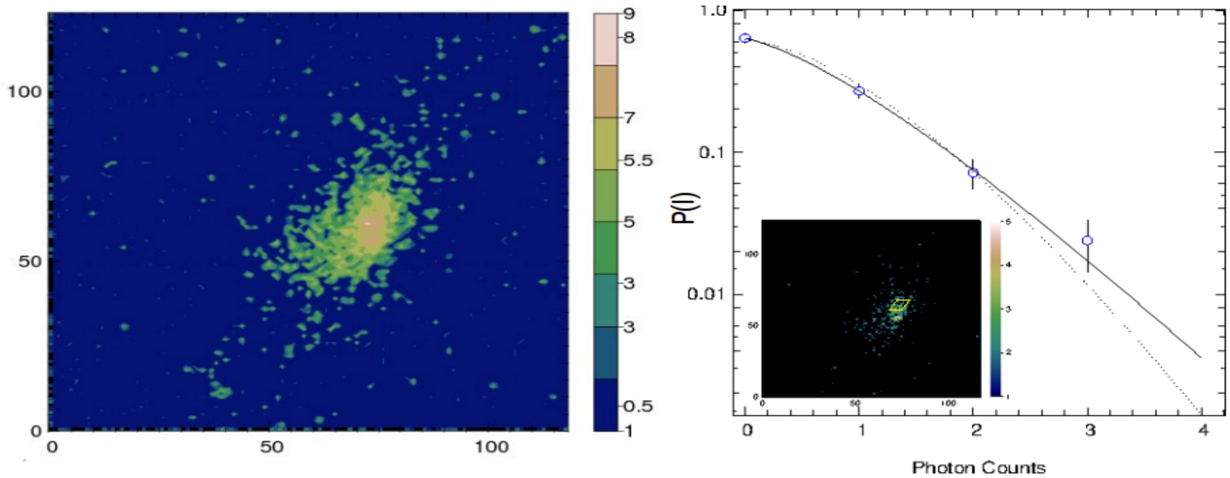


Figure 1 Speckle patterns near the (409) Bragg reflection from a conA crystal (left); Right: Speckle intensity distribution: probability of detecting 0,1,2,3 or 4 photons/s/pixel in a small region of the reciprocal space shown in the inset. The intensity histogram resulting from noise in the detected signal is expected to follow a Poisson distribution (dotted line). The measured intensity distributions are better fitted by a negative binomial distribution showing evidence of speckles obtained with a coherent beam.

The experiments faced several technical hurdles associated mainly with the need of switching between a PX experimental setup to one for measuring diffuse coherent scattering. No existing beamline can provide such capabilities in an efficient way, but the future CHX beamline at NSLS-II (one of the six initial project beamlines) will provide such unprecedented capabilities in a user-friendly way. An essential part of this project consists in developing the systems and the capabilities of repeating the same measurement at different locations on the sample. This will allow to reduce the error bars in measurements such as the ones shown in Figure 1. For this purpose we built and tested an on-axis sample visualization microscope. In Figure 2 we show some experimental results obtained with this microscope.

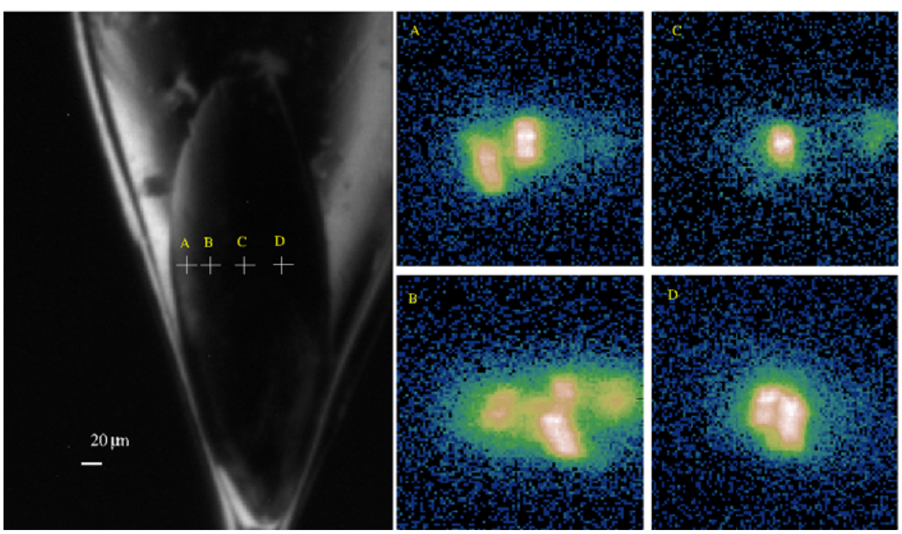


Figure 2 Example of coherent microbeam diffraction from flash frozen Hb crystals. An on-axis microscope allows choosing the precise location of the beam on the sample. Complex diffraction patterns (integrated rocking curves) recorded from the four locations shown here provide evidence for the existence of several microdomains (mosaicity) most likely created by the freezing procedure.

The main focus during the next following moths will fall on writing several publications based on these results and on preparing the "transfer" of all the experimental techniques developed here to the future research program of the CHX beamline.

High-Resolution Biological Imaging by X-ray Diffraction Microscopy

LDRD Project 11-027

Enju Lima

PURPOSE:

High-resolution biological imaging is challenging, however, when successful its impact on life science is extremely fruitful. While electron microscopy (EM) delivers nanometer resolution with thin samples less than a micron in thickness, larger samples need to be cryo-sectioned, at the cost of potential artifacts or experimental difficulties, in order to achieve high resolution. The current proposed LDRD explores the feasibility of x-ray diffraction-based imaging of biological samples in the frozen-hydrated state. Utilizing the high-penetration power of x-rays and algorithmic computation, it aims to overcome the current limitations of x-ray optics resolution and the sample thickness limitations in cryo-EM.

APPROACH:

Frozen-hydrated biological imaging by hard x-ray diffraction microscopy was previously demonstrated in two dimensions by the PI and collaborators. Further advances, including higher resolution and 3D imaging, have not yet been demonstrated despite ongoing efforts. The current LDRD of "High-resolution biological imaging by x-ray diffraction microscopy" is exploring high-pressure cryogenic sample preservation in order to improve the success rate. The project is also developing a method to expand the scope of cryo-XDM to image extended biological samples of tens-of-microns in size.

TECHNICAL PROGRESS AND RESULTS:

1. High-pressure cryo-preservation method was adopted for cryo-XDM. The work is in collaboration with C. Kim and S. Gruner at Cornell University and P. Pernot at ESRF, France. Part of the work was summarized by Chae Un Kim, Jennifer L. Wierman, Richard Gillilan, Enju Lima and Sol M. Gruner in the paper "**A high-pressure cryocooling method for protein crystals and biological samples with reduced background X-ray scatter**" which is currently *in print* with Journal of Applied Crystallography.
2. Multiple reconstructions of frozen-hydrated *D. radiodurans* bacteria were obtained using high-pressure cryo preservation to reach ~25 nm resolution in two dimensions, exceeding the resolution of hard x-ray optics. A manuscript is under preparation.
3. Cryogenic scanning x-ray diffraction microscopy was developed by the PI and collaborators at Swiss Light Source during FY11 and FY12 to expand the scope of XDM to larger samples. The work was summarized by E. Lima, A. Diaz, M. Guizar-Sicairos, S. Gorelick, P. Pernot, T. Schleier, and A. Menzel in the paper "**Cryo-scanning x-ray diffraction microscopy of frozen-hydrated yeast**" published in Journal of Microscopy, December 2012.
4. A post-doctoral fellow, Li Li, was hired in FY12 and has continued on the project. Based on his experience with crystal diffraction, Bragg x-ray diffraction microscopy was added as a part of LDRD. Crystal coherent diffraction simulation was carried out during FY12 and manuscript preparation continues in FY13.
5. Computer software for diffraction data assembly is being developed for 3D imaging of biological samples.

Milestones for each year of anticipated funding.
FY13:

- Publication of 2D high-resolution imaging of high-pressure-frozen, hydrated *D. radiodurans*
- 3D reconstruction of frozen-hydrated *D. radiodurans*
- Publication of a crystal coherent diffraction simulation

Sub-10 nm Resolution Soft X-ray Microscopy of Organic Nano-materials by Novel Diffraction Methods

LDRD Project 11-030

K.Kaznatcheev

PURPOSE:

The spatial resolution of x-ray microscopy is limited by the performance of the x-ray optics to ~20nm, which corresponds to numerical aperture of 0.03 for 1nm soft x-ray radiation. At the same time, specimen scattering cover much larger cone, and, particular for a moderately radiation tolerant colloidal nano-particles assembly, is often extended to a Q range of $1nm^{-1}$ at normal (1s per frame) acquisition speed. If x-ray light is coherent, one can apply a Fourier inversion (FFT) of x-ray scattering pattern to find the real space distribution of scatters. The problem is to find a proper set of scattering wave phases, as only modulus of FFT is know from scattering intensity. The input-output iterative algorithms are found to be capable of real space reconstruction of scattering fields with minimal assumptions regarding specimen structure. Fueled by the recent development of coherent x-ray sources (such as NSLS-II), diffraction imaging has a potential to become a technique of choice for x-ray high resolution imaging. LDRD11-030 is focused on the development of experimental and computational techniques which permits imaging of organic nano-materials at the spatial resolution exceeding diffraction limited performance of state-of-the-art x-ray optics and it has two aims: (i) development of quantitative ptychography and (ii) follow up investigation of meta-materials (high-resolution structure of the Au/DNA crystals in various states of self-assembly) .

APPROACH, TECHNICAL PROGRESS AND RESULTS:

The recent development of scanning coherent x-ay diffraction microscopy (also known as ptychography) eliminates several constraints exerted by coherent imaging. In particular, an illuminating wave (the probe) can have an arbitrary shape, as a diffraction data redundancy due to multiple measurements at overlapping neighboring probe positions permits its independent reconstruction along with the scattering potential (the object wave). A priori knowledge, such as a finite sample support, is reduced to a recording of sequential probe positions and a plausible guess to be used as a starting estimate for iterative phase retrieval. Using a focusing probe, such as one produced by a zone plate, we investigate the effectiveness of the reconstruction algorithm and find that it is significantly less successful at reconstructing wave-fronts with large curvature (extended phase variation) than the wave-fronts with almost flat phase structure. Our simulations show that when the actual probe has large phase variation, the amount of overlap required for a successful reconstruction of both object and probe depends upon the phase difference between the actual probe and the probe used as a starting estimate for the reconstruction [S.Wang, et al., x-ray ptychography with highly-curved wavefront, submitted]. Aimed with simulation results we have optimized the experimental procedure, and as illustrated by Fig.1(b) reaches spatial resolution beyond diffraction limited performance of x-ray microscopy (Fig.1(a). We also went beyond measurements of lithographically made nano-structures and were successful in reconstruction of thin NP film at 5nm nominal resolution (Fig.2). Although that constitute the

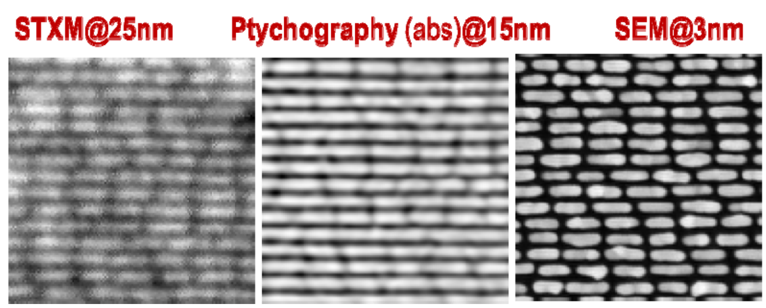


Fig.1. Imaging of zone plate outermost area (20nm of 80nm thick Au lines) by different techniques, total dose ~equivalent ($10^9 ph/um^2$), step 5nm.

goal of LDRD, the robustness of image reconstruction still remains a pressing issue and we proceed with two important developments described below.

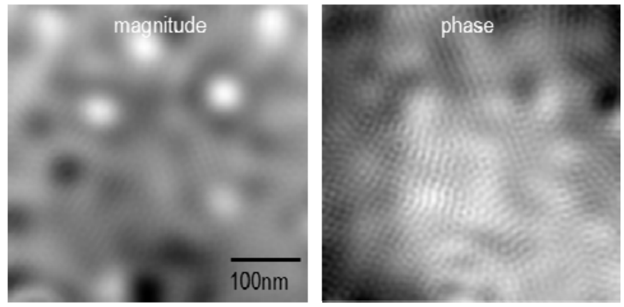


Fig.2. Ptychographic reconstruction of NP thin film. NP (Fe_2O_3 :12nm) positions can be derived from high frequency phase modulation, although low frequency background variation is likely to be artificial.

Measurement of the optical transfer function (OTF) as a system spatial frequency response remains at the heart of the characterization of any imaging system or technique. It not only provides a thorough quantitative measurement of amplitude modulation and phase delay but also reveals (i) characteristic noise due to detector performance or system mechanical instability and (ii) deficiencies of the image data processing as a part of the reconstruction algorithm. We have developed special WSi2/Si multilayer sample where the layer structure follows a pseudo-random binary sequence with a fundamental layer thickness of 3 nm as a calibration standard. As the spatial frequency response of such sample has flat power density spectra till 2π/3nm cutoff it makes easy for experimental data to be normalized. Data collected at different energies and illuminations show complex behavior with the power spectrum extended to ~nm^{-1} and largely limited by CCD dynamic range at a dwell time of ~300 ms. Coherent diffraction imaging returns both specimen transmission amplitude and phase, and one can compare the absolute value of the OTF, also known as the modulation transfer function, as one measured (a) directly from an angular extension of the speckle cone averaged over the sample length, or (b) from a reconstructed image. The article detailing cross comparison of those two approaches and a further framework for quantitative definition of sample reconstruction accuracy is under preparation.

Materials that lack long-range translational order present a substantial difficulty for characterizing their "atomistic" structure. As a result, property-to-structure relation for glasses, gels, foams or colloidal crystals are not well established. Coherent x-ray scattering speckle pattern uniquely defines a spatial distribution of scatters and the recent development of coherent diffraction imaging (CDI) is meant to be a route for reconstruction of their spatial distribution. Unfortunately, even with the development of ptychography - a robust image reconstruction technique not limited by isolated specimen requirement or a priori knowledge of incident illumination - real experiments often fail, especially when only incomplete (with missing portion of Q space) or noisy data set are available. If one is primarily interested in symmetry of scatters local arrangement, a full CDI inversion is not needed and parameters of hidden structural ordering can be revealed by employing x-ray cross-correlation analysis (XCCA) directly to the speckle map. Smaller spot size (fewer effective scatters probed) help to divulge distinct angular correlation even for a disordered structure, where a raster scanning provide needed statistical averaging over the large ensemble. As XCCA is done on a point-by-point basis, the spatial distribution of particular structural motif can be mapped this way. Alternatively, one can measure a decrease of angular correlation XCCA as probe size increases (as in fluctuation microscopy) to extract the spatial extent (correlation length) of distinct structural motifs for a given specimen point. Using a dense nano-particle 2D assembly, as a model system, we have developed experimental techniques for accurate and systematic characterization of disordered systems.

2D Membrane Solution Scattering for Probing the Structures of Membrane Proteins

LDRD Project 11-032

Lin Yang

PURPOSE:

This LDRD project aims to develop the experimental methods needed to utilize X-ray scattering to study the structure of membrane proteins embedded in single-layered lipid membranes that resemble the native environment of these proteins. While this technique has never been demonstrated, we have already obtained similar results on plant viruses (much larger than membrane proteins and therefore easier to measure). The difficulty is to collect high quality data free of background scattering and without introducing radiation damage to the proteins, which we will overcome by flash freezing the membrane sample and performing the measurements at liquid nitrogen temperature.

APPROACH:

Structural determination of membrane proteins is a grand challenge in structural biology. A key limitation in these studies is that the membrane proteins must be extracted from membranes using detergents, so that the resulted soluble protein-detergent complex can be studied using methods available for soluble proteins. Unfortunately, the presence of detergents creates some detrimental side effects. Measuring the membrane proteins in substrate-supported, single-layered lipid membrane that mimic the proteins' native environment is a promising alternative. The membrane sample can be created under well-defined chemical conditions that are required for the proteins to function. However, in order to apply this method to membrane proteins, the sample must be exposed to X-ray for long periods of time, implying higher probability of radiation damage to the sample.

Under this project, we will develop methods to flash freeze the membrane samples and measure them at liquid nitrogen temperature. It is known that radiation damage due to the diffusion of free radicals can be dramatically reduced at low temperatures. Once the membrane sample is frozen, it will also be possible to remove the substrate on which the membrane structure is created. Doing so will expose the membrane structure directly to the X-rays, thus virtually eliminating the background scattering from bulk water. This effort is in collaboration with Masa Fukuto of CMPMSD and Dax Fu of Biology Department.

TECHNICAL PROGRESS AND RESULTS:

During FY12, we completed the slam-freezing instrument (Fig.1) and tested lipid monolayer samples supported on 50μm thick silicon substrates coated with hydrophobic silane molecules. The samples were prepared following the same procedure that was established for virus samples on thicker substrate in room temperature experiments. The sample is then mounted at the end of a linear motor that rapidly moves toward a polished cold copper mirror located in the cryostat and surrounded by dry nitrogen gas. The gate valve on the cryostat is then closed to allow the cryostat to be evacuated and the grazing incident X-ray scattering measurements are performed on the frozen sample through the windows on the cryostat.

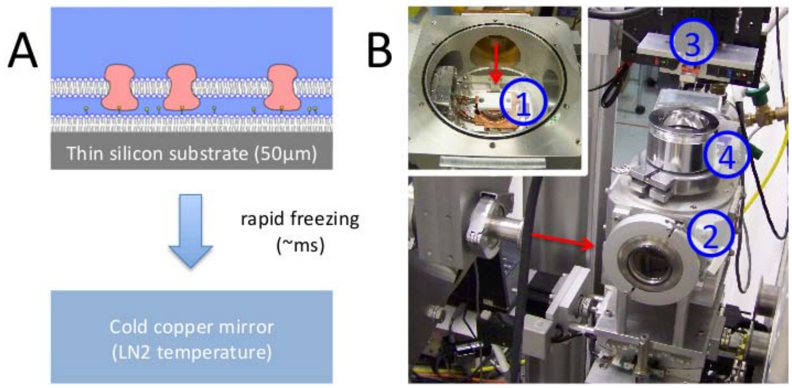


Figure 1 (A) A schematic illustration of rapid freezing of lipid membrane structures supported on a thin substrate. Vitreous ice is expected to form within the layer above the substrate that is tens of microns thick and much thicker than the membrane structure itself (~10nm). (B) The actual instrumentation at beamline X9 of NSLS. The inset shows the details inside the cryostat. The labeled components are (1) sample, (2) cryostat, (3) linear motor, and (4) gate valve.

In order to understand how to create vitreous ice for the purpose of preserving sample structure and reducing background scattering, we studied the wide-angle diffraction data from samples that contain various concentrations of cryo-protectants (PEG). We confirmed that PEG indeed help to form vitreous ice, and that ice amorphous ice formation is more pronounced near the substrate, where the cooling rate is higher (Fig.2). However, we also learned that at small scattering angles, the scattering intensity from ice is still significantly higher (data not shown) than that from the membrane structure that is actually of interest. We also found that this small angle scattering intensity can vary from sample to sample, due to minor inconsistency between individual freezing operations.

It is becoming clear that more radical approach is needed in order to accelerate the cooling rate of the sample and to improve the reproducibility of the freezing procedure. We are now working on a new apparatus that have several improvements over the current design. Instead of freezing the sample through the substrate, we mount the substrate on the cold stage. The sample is prepared on a Langmuir monolayer on the surface of the solution in the sample cell instead. Therefore, we expect to achieve significantly higher cooling rate by making direct contact between the membrane structure and the cold surface. Having the sample on a fluid surface also makes it easier to align the apparatus. The cold surface is shielded from the sample until the final contact to avoid pre-cooling of the sample and again increase the cooling rate of the sample.

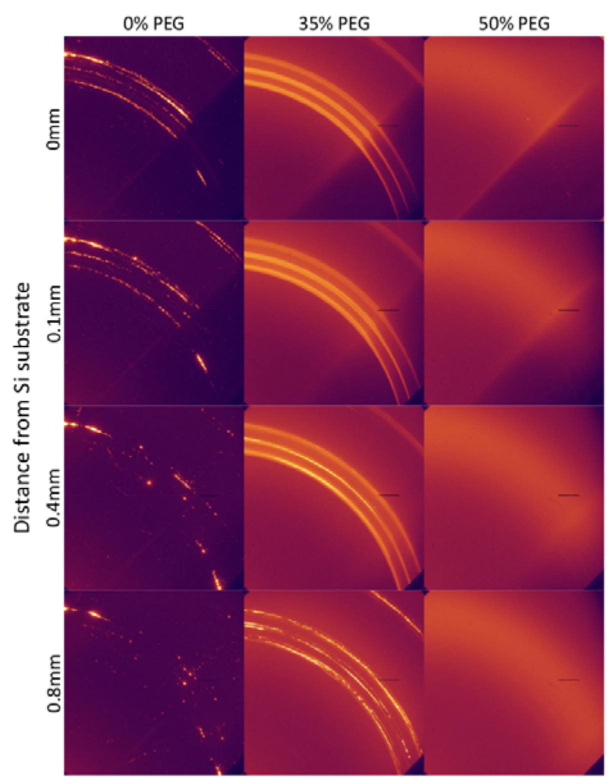


Figure 2 Grazing incident diffraction data from the frozen samples at various PEG concentrations. The diffused peak at

For the remainder of the project, we plan to continue the development and tests of the experimental apparatus. We still aim to obtain high quality data from streptavidin, a model membrane protein, by the end of the project. If this is successful, we will shift our focus to analyzing the scattering data and measurements of actual membrane protein supplied by Dax Fu's group.

Exploring the Role of Glue in Hadron Structure by an Electron Ion Collider

LDRD Project 11-033

Jianwei Qiu

PURPOSE:

After almost 40 years' successes of Quantum Chromodynamics (QCD) in interpreting the data from high-energy collisions, we only know very little on how the quarks and gluons make up nucleons and nuclei. Since the current quark mass for the light quark sector of QCD is so much smaller than the mass of nucleons, it is the glue that binds matter into strongly interacting hadronic particles. The proposed eRHIC by BNL with both e+p and e+A capability could be a powerful femtoscope (or even an attoscope) to explore the quark-gluon structure of hadrons and nuclei. The goal of this LDRD project is to identify a set of semi-inclusive observables in e+p and e+A collisions that could provide the direct access to the glue content of a hadron or a nucleus and to explore the role of glue in forming stable hadrons or a nucleus. Our investigations focus on two types of observables: jets and heavy flavor production in the DIS regime of both e+p and e+A collisions. The knowledge gained from this project could help articulate the physics case as well as machine parameters of a future eRHIC.

APPROACH:

Data from HERA – an electron proton collider at DESY, Germany, demonstrated a very strong growth of the number of soft gluons inside a proton. Since the growth is so strong that it could lead to a violation of the Froissart's unitarity bound on hadronic cross sections, soft gluons in a hadron must interact with each other strongly and coherently. The interaction and the coherent strong color field dynamics in QCD could lead to a novel form of saturated gluonic matter, referred as the "Color Glass Condensate" (CGC). Since gluon does not carry electromagnetic charge, it is dark and cannot be "seen" directly by the electron beam at eRHIC. It is therefore very important and necessary to identify observables that are sensitive to the role of gluons inside the colliding hadron while visible to the colliding electron beam.

It is the quark or antiquark (heavy or light) that carries both electromagnetic charge and color charge, and can bridge the interaction between the probing electron beam and the glue of a hadron. With a large momentum transfer, glue interacts with the colliding electron at the *short distances* via a highly virtual light quark or antiquark, which has a characteristic event structure with two nearly back-to-back jets in the Breit frame. At a relatively small x_B, the two-jet final-state should be an excellent observable to directly probe the gluon content of the colliding hadron because of the dominance of photon-gluon subprocess. Our goal is to calculate the jet cross section in the semi-inclusive deep inelastic scattering (DIS) at eRHIC. The result for e+p collision provides a unique tool for measuring the gluon content of a proton, while the jet modification in e+A collision provides a more direct way to explore the properties of the glue and color structure inside a heavy nucleus.

In addition, the production of heavy quarkonia at eRHIC could be the most sensitive and controllable observable for probing the glue, in particular, its non-linear QCD dynamics in the transition region when the gluonic matter enters a new CGC domain. To the first approximation, the photon-glue fusion is the only channel to produce a heavy quark pairs necessarily needed for producing a heavy quarkonium. Unlike the light hadrons or jets, a heavy quarkonium has multiple distinctive momentum scales: heavy quark mass, confined momentum, and binding energy. Heavy quarkonium production at eRHIC could be an excellent laboratory for investigating the dynamics of color neutralization as well as the production mechanism of a QCD bound state where the major contribution to its mass is from the quark not from the energy of gluons. Our goal is to develop the correct formalism for calculating the cross section of heavy quarkonium production in high-energy collisions. In particular, at eRHIC, we explore the role of color and quark mass in the formation of a color singlet and bound heavy quarkonium.

TECHNICAL PROGRESS AND RESULTS:

Fiscal year 2012 was the second year of this project. Since January 1, 2011, a graduate student of Stony Brook University, Mr. Hong Zhang, has been supported by this LDRD grant, who is working on quarkonium production for his Ph.D. thesis. In addition, since August of 2011, a postdoc, Dr. Yang-Qing Ma joined the project. A complete list of publications and presentations in connection with this project is given in a separate LDRD Data Collection Form.

The student, Mr. Zhang, just finished a set of very difficult and the first ever calculations of transition probabilities for perturbatively produced heavy quark pairs in high-energy collisions to transmute into non-relativistic heavy quark pairs in all possible spin and color states. These transition probabilities are necessary for making precise predictions of heavy quarkonium production. His results are being checked, and papers are being prepared in order to publish these very important results. These results should form the main part of his Ph.D. thesis.

The postdoc, Dr. Yang-Qing Ma, is the best theory postdoc working on physics of heavy quarkonium production in the world. His complete next-to-leading order predictions, the first in the world, have been recognized world wide as the standard QCD predictions and were compared to data from the B-factory, RHIC, Tevatron, and the LHC. While at BNL, Dr. Ma and his collaborators proposed the first creditable solution for the long-standing polarization puzzle in J/ψ production at collider energies. He is now working full time on the quarkonium production and signatures at a future eRHIC, and is finishing up two more papers with the PI of this project. In addition to work with the student and the postdoc on heavy quarkonium production, the PI has been collaborating with experts around the world to investigate the role of jet production in probing the glue as well as the spin physics in connection with this project. In the rest of this two-page report, we highlight two of those published works.

With Dr. Kang of Los Alamos National Lab and Prof. Sterman of Stony Brook University, we developed and proved a new QCD factorization formalism for heavy quarkonium production in high-energy collisions. Our work provides new physics insights on how a physical quarkonium is produced in high-energy collisions, which is very important for understanding heavy quarkonium production at eRHIC. The first part of our work has recently been published in Physical Review Letters [108 (2012) 102002], and more results are being prepared for publications. Dr. Ma, the postdoc on this project, is now a new member of the team and is taking the lead of our effort on heavy quarkonium production.

With Dr. Kang and Dr. Mantry of Argonne National Lab, we proposed a new observable, referred as Jettiness, to better probe the nuclear effect in electron-ion collisions at eRHIC. As a measurement of N-jet event shapes, the Jettiness carries the same advantage of jet production for probing short-distance dynamics, while its inclusiveness provides a much better measurement on nuclear modification in comparison with the well-known “jet-quenching” observable, which is too sensitive to the jet definition. The first paper on this effort was published [Phys. Rev. D86 (2012) 114011. More results are expected and will help support the eRHIC.

CMOS-Pixel Vertex Detector for EIC

LDRD Project 11-036

Elke-Caroline Aschenauer and Benedetto Di Ruzza

PURPOSE:

BNL is working on the design of a new accelerator; this new accelerator will add an electron machine to the existing hadron machine at RHIC. This will be the most cost effective solution for an electron ion collider (EIC) in the US. A dedicated detector for EIC should include a vertex detector that can track over a wide range of pseudo-rapidity and down to the lowest p_T allowed by the detector geometry and needs to be capable of reconstructing displaced vertices from heavy flavor decays.

Traditionally, such detectors are implemented in two separate parts – a "barrel" layer that detects tracks out to $|\eta| \sim 1$ and an "endcap" composed of disks that extend the acceptance down to smaller polar angles (larger $|\eta|$). To achieve the performance needed to resolve displaced vertices from the primary vertex down to distances of < 100 μm, the barrel and end-cap will need at least three sensitive layers providing two-dimensional measurement of particle positions with resolutions <10 μm in both directions. The traditional choice of technology for vertex detectors designed to measure heavy flavor decays is silicon hybrid pixel detectors.
Such detectors were tested for the first time in the WA97 [1] and DELPHI [2] detectors. Today they are an integral part of the tracking systems for any particle detector, i.e. ATLAS, CMS and ALICE at CERN.

However, such detectors used in the LHC experiments, typically contain a layer of 100-300 μm of silicon as sensor and significantly more material in the separate readout chips resulting in typically ~ 3% - 10% radiation length of material per layer. Detectors based on such design, are unsuitable for EIC applications where the energy of the scattered electron is much lower than the energy produced in the LHC machine. In an EIC machine – at least in the barrel and in the backward (electron beam direction) endcap detectors, the constraints on material budget necessary to limit electron bremsstrahlung are more severe than in a proton/proton high-energy machine. That is why an EIC machine require devoted research and design for the tracking; it's not possible to simply reuse the ongoing research already done for a LHC type machine.

In the last decade there has been significant progress in the development of Monolithic Active Pixel Sensors (MAPS) in which the active detector, analog signal shaping, and digital conversion take place in a single silicon chip (i.e. on a single substrate) (see [3], [4] and references therein).
These devices built using CMOS technology use an epitaxial layer as the active sensing element.
Ionization deposited in the epitaxial layer is collected by N+ wells embedded in the epitaxial layer. The "pixel" pitch is determined by the location of the N wells so there is no need for actual segmentation of the detector as in traditional hybrid pixel detectors. As a result, CMOS pixel detectors can be built with very high segmentation, limited primarily by the space required for additional shaping and digital conversion elements. Present technology allow to a resolution of 20x20 um.

Brookhaven National Laboratory, Columbia University and IPHC-CNRS started a research program in order to investigate the use of silicon pixel MAPS sensor "MIMOSA" type, designed in the Institut Pluridisciplinare Hubert Curien (Strasbourg, France), for the μ−vertex for a new dedicated EIC detector.

MAPS μ−vertex detectors in the barrel of particle detectors have become more common, but the unique development of this research will, for the first time, produce a prototype MAPS μ−vertex detector disc for the endcaps of the detectors. In addition a test stand for MAPS is to be realized at BNL. This should be the place to test small prototype sensors and achieve the know-how required to design the global pixel detector for the EIC detector.

The main risk of this research lies in realizing a technology called stitching to combine chips in quadrants, which will be used to form the forward discs. This technology has till today never been realized.

The present goals of this research are:

1. Test the limits of the read-out speed of different prototype models (such as Mimosa26, Mimosa28 and the future Mimosa32) in order to establish, which is the best model prototype for an EIC detector.
2. Test how the performance of the different chips changes as function of temperature
3. Test one sensor of the new more radiation hard sensor technologies, i.e. Mimosa32, still under development, in a light source line in order to emulate the background condition of EIC detector.
4. Integrate a detector into the GEANT model of the EIC detector and study the number and placement of the forward discs needed to achieve the desired tracking resolution.
5. Further study integration issues of the detector so close to the beam line to understand air-cooling would be an option.

APPROACH:

For this project a post-doc position was opened and Benedetto Di Ruzza was hired in this position. Benedetto di Ruzza worked since 2004 in the CDF collaboration at Fermilab, taking care of the monitoring of the secondary vertex online trigger (SVT [5], then GigaFitter [6]) and doing B physics analysis for his Ph.D. thesis. In 2009 he became member of the CDF Silicon Operation Group, and since August 2010 he is one of the two Project Leader of the CDFII Silicon Operation Group. He has a large experience in silicon detector operation [7] and maintenance [8].

In BNL the main task of this research is develop a test-stand station in order to test the “Mimosa sensors” with a laser source, cosmic rays and radioactive sources (^{55}Iron and ^{90}Strontium). The starting point of this test stand is the hardware and software setup already used at DESY and CERN in the “EUDET Beam telescope” (Mimosa-26 sensors with LabVIEW based data acquisition system [9]) designed for a “Linear Electron Collider type” silicon tracker develop.

At BNL the “EUDET DAQ system” will integrate a temperature monitor in order to control the efficiency of the sensors at different temperatures, because the MAPS sensors collects the signal using thermal diffusion, instead of bias depletion voltage such us in the Atlas and CMS sensors. In a MAPS sensor an increase of temperature decreases the collection time, but increases the noise, that’s why it is important to find the best equilibrium point for every different chip design.

All this work is performed together (web meetings weekly planed, discussions, exchange of tools and experience, travels etc.) with the Group of Prof. E. Hughes and Prof. B. Cole at Columbia University and the IPHC-CNRS Group at Strasbourg. For the BNL laser station set-up an undergraduate student from Stony Brook University was hired in the 2013 winter break. The plan for the future is to try to involve new Stony Brook Students using the educational programs already available in BNL.

The latest results achieved together with the Columbia Group and the Strasbourg Group were presented in the 2012 IEEE NSS conference (Anaheim, CA, October 2012). Another key work that will be performed at BNL will be the detailed GEANT simulation of all these different silicon sensors prototypes in realistic electron-proton/ion collisions. This work will be performed in collaboration with a new post-doc already hired here in BNL for the EIC simulations. These simulations will give us precise constraints on the type of detector geometry possible.

A first meeting on the EIC simulation was performed here in BNL [10] and the general detector simulation framework was chosen.

It is very important to remember that all this R&D work, even if mainly oriented for a EIC collider detector, can be used in a wide range of other applications: first of all, new medical tracking sensors, but also homeland security tracking sensors.

The main advantages of the Mimosa sensor are that it is very cheap to produce, easy to handle, sensitive to both gamma rays and radioactive particles. That's why it is important to establish in BNL a test-station for this sensors and the basic know-how about this technology to apply this sensors to present and future strategic targets.

TECHNICAL PROGRESS AND RESULTS:

At Columbia University in the last year a test stand was realized mainly oriented to laser tests of the Mimosa chip. It includes a standard "EUDET type Mimosa26" DAQ system, a 1060□m laser and the possibility to scan the surface of the silicon sensors in x-y in steps of 10 microns, (same size as the pixels), and two 40dB light attenuators. These possibilities are also realized at BNL. The test stands are able to perform a read-out with a fixed trigger rate, but also with random (laser) input using a special DAQ board. The same board will also allow us to trigger on cosmic rays and radioactive source signals triggered by a PMT. A laser profiler will allow measurements of the collection efficiency of silicon sensors of the same family.

Two important studies already performed by under-graduated and graduated students in the Columbia group are:

1) Study of the uniformity of a Mimosa-26 prototype
2) Study how changing the laser profile influences the threshold noise for the same prototype.

At BNL the next step is to test Mimosa-28 and Mimosa-32. In order to do this, Benedetto Di Ruzza will stay for 4 weeks in Strasbourg in order to collaborate with the designers on how to handle these sensors. After this, in July 2013, we expect to do a test-beam on the new silicon prototype Mimosa-32 at DESY. Benedetto Di Ruzza, and most likely some BNL/Stony Brook/Columbia University students will participate.

[1] F Antinori et al. Experience with a 30-cm silicon pixel plane in CERN experiment WA97. NIM A360 (1995) 91.
[2] A. Andreazza et al. The DELPHI very forward tracker for LEP-200. NIM A367 (1995) 198.
[3] R Turchetta et al., NIM A 458 (2001) 67.
[4] Marc Winter for the IPHC-IRFU collaboration, NIM A 623 (2010) 192.
[5] J. Adelman *et al*., Real Time Secondary Vertexing at CDF, Vertex 2005, Nikko, Japan, NIM A569 (2006) 111.
[6] CDF Public Note Number: CDF/DOC/TRIGGER/CDFR/10030.
[7] International TIPP conference Chicago 2011
http://indico.cern.ch/getFile.py/access?contribId=148&sessionId=22&resId=1&materialId=slides&confId=102998
[8] http://detectors.fnal.gov/EDIT2012/participants.html
[9] http://indico.cern.ch/conferenceDisplay.py?confId=89979
[10] EIC R&D Simulation workshop (BNL October 8th -9th 2012)
https://wiki.bnl.gov/conferences/index.php/EIC_RD_Simulation/Agenda

Study of FEL Options for eRHIC

LDRD Project 11-040

Vladimir N Litvinenko

PURPOSE:

Potential performance of X-ray FELs driven by eRHIC's high-energy electron ERL was studied since 2004 and recently returned to the focus as potential future direction for BNL's light sources. This project will be focused on detailed studies of various X-ray FEL options for eRHIC including single pass SASE FEL, seeded and HGHG FELs, and X-ray FEL oscillators. Advanced FEL and beam dynamics codes will be used to evaluate various FEL options, compare them and connect them to potential applications

APPROACH:

The goal of this LDRD project is to explore the potential of eRHIC as a driver for a farm of X-ray FELs as well as a driver for an X-ray FEL oscillator. During this fiscal year we focused on an advanced version of the eRHIC driven FEL – X-ray optics-free FEL oscillator (OFFELO).

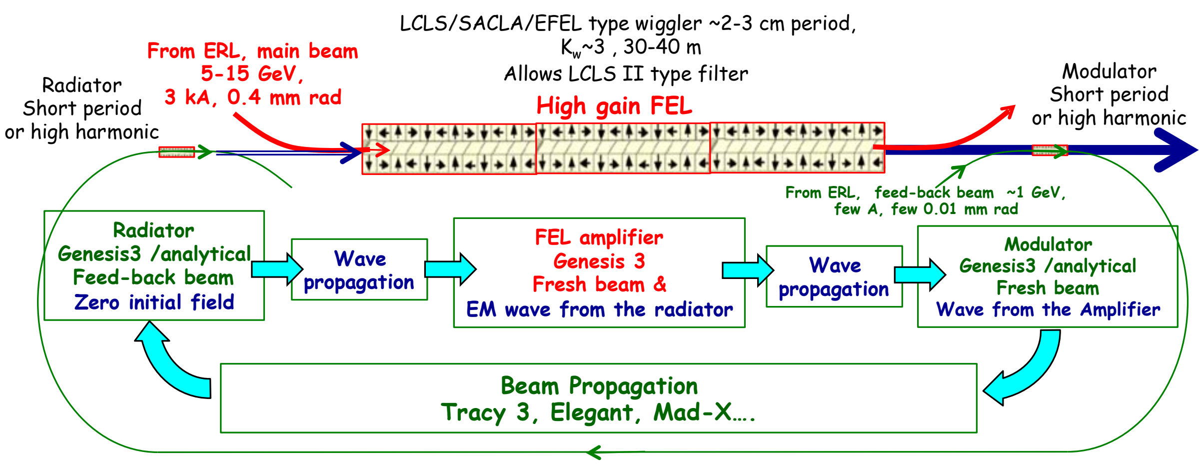


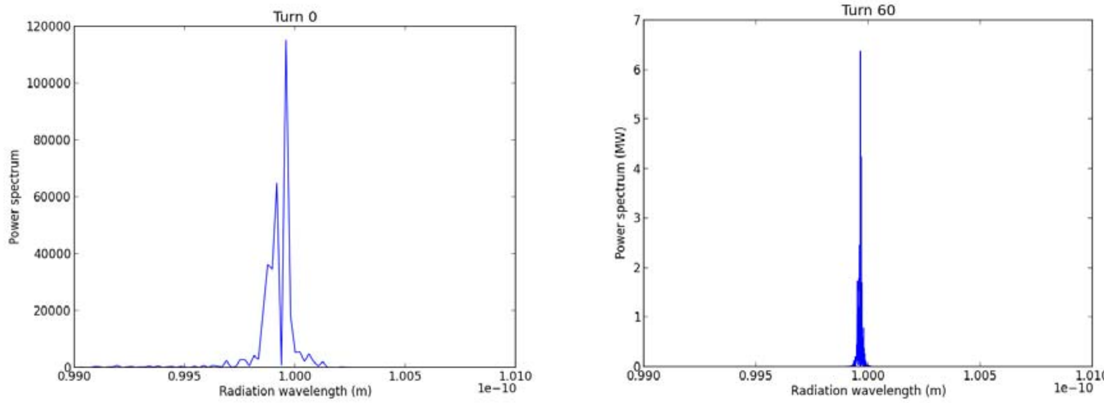
Fig. 1. Schematic layout of possible eRHIC-based OFFELO

TECHNICAL PROGRESS AND RESULTS:

We continued developing the FEL farm approach as well. The main load was carried by Dr. Y. Jing selecting bam parameters and bunching scheme for X-ray FEL farm.

CSR is one of the main limiting factors for most of advanced X-ray FEL schemes. We investigated schemes of suppressing CSR in X-ray FEL zig-zag compressors as well as passive ways of CSR shielding. Results of experimental demonstration of CSR suppression by conducting plates were published in PRL [1]. Yichao Jing gave a talk at CFA Workshop on Future Light Sources on novel FEL zig-zag compressor scheme and submitted paper to FEL proceedings and PR ST-AB [2-3].

During this fiscal year a rather large team of scientists from C-AD and NSLS II (J. Bengtsson, Y. Hao, Y. Jing, D. Kayran, VL and D. Trbojevic) focused on start-to-end simulation of the X-ray FEL oscillator – including detailed development of the lattice and tracking. We developed two schemes and demonstrated preserving of the correlation at sub-angstrom level in an electron beam traveling through 300 m and 3 km long arcs. A complete set of program was developed to close the OFFELO loop and to study the evolution of its radiation spectrum. A typical example is shown in Fig. 2. We also started studies of collective beam effects – such as CSR- in the OFFELO, and defined necessary remedies.



(a) (b)

Figure.2. Evolution of the radiation spectrum in OFFELO (a) Starting of OFFELO lasing – SASE spectrum after first pass (b) Spectrum of OFFELO after 60 passes with RMS bandwidth of 0.01%.

Results of these studies were presented as an oral talk at the FEL 2012 conference and were published. A manuscript for a refereed journal is under preparation for submission in early 2013.

FEL options for eRHIC were the topic of frequent discussions and presentation at Doon Gibb's AST meetings during FY12.

We plan to finish all remaining simulations and compile the final report in first half of 2013.

Publishing submitted a refereed paper on zig-zag FEL bunch compressor, as well as publishing a refereed paper on OFFELO will complete this LDRD research.

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Overcoming Electromagnetic Interference in Simultaneous PET and MRI for Biological and Clinical Imaging

LDRD Project 11-050

Paul Vaska, David Schlyer, Craig Woody

PURPOSE:

Recently the concept of acquiring positron emission tomography (PET) images simultaneously with magnetic resonance imaging (MRI) has generated considerable excitement in biomedical science. The new possibilities engendered by this fusion of two distinct but complementary imaging modalities are numerous in medicine, relating to the accurate image alignment between the functional image and its anatomical reference frame, and to the potential for interrogation of multiple functional measures simultaneously using functional modes of MRI such as fMRI, spectroscopy, or diffusion tensor imaging. Further, this approach is being applied to the broader context of biological imaging, in particular, to understand basic biochemical mechanisms in plants in an effort to develop improved biofuels and to predict the impact of climate change on critical plant species. Our group has been one of the pioneers in the area of multimodality PET-MRI imaging, having developed modular PET detectors and prototype imaging systems that can tolerate the punishing MRI environment which consists of strong static and dynamic magnetic fields and high power radio-frequency transmission. However, the integration of the two systems has been challenging, in particular, due to the interference between the modalities each of which rely on high fidelity radio-frequency electromagnetic signals. In our prototype systems, significant interference has been observed in both PET and MRI data despite initial attempts at isolating them with electromagnetic shielding. In this proposal, we plan to investigate the generation and propagation of the electromagnetic interference (EMI) in a rigorous and methodical manner, and to develop and test technological approaches to mitigate the problem to the greatest extent possible. This will build a foundation for multiple ongoing and planned projects in simultaneous PET and MRI imaging.

APPROACH:

We aim to analyze the potentially deleterious signals in the relevant PET and MRI subsystems, and then develop ways to shield or otherwise mitigate the effects. This includes analysis of the sources of electromagnetic waves, the transmission paths, and the circuits that are sensitive to them. Building upon this analysis, we will design and test optimized electronics and various shielding configurations.

TECHNICAL PROGRESS AND RESULTS:

We have built various radiofrequency (RF) shield configurations for our MR-compatible PET system as shown in Fig. 1, as well as RF transmit and receive coils and coil shields appropriate for that system. We analyzed the effects of RF pulsing on PET count rates under various MRI pulse sequences as shown in Fig. 2 (left). Without any shielding, there are large background rates generated in the PET electronics. The solid aluminum shield provides the best RF protection and the segmented shields less so. However, as shown in Fig. 2 (right), the solid shield induces severe artifacts in the MRI images. The main conclusion is that the current segmented shield provides the best balance of noise suppression and MRI image quality.

Some of the funding was used to procure more of our specialized MR-compatible electronics, specifically our application-specific integrated circuit (ASIC), so that this work could continue.

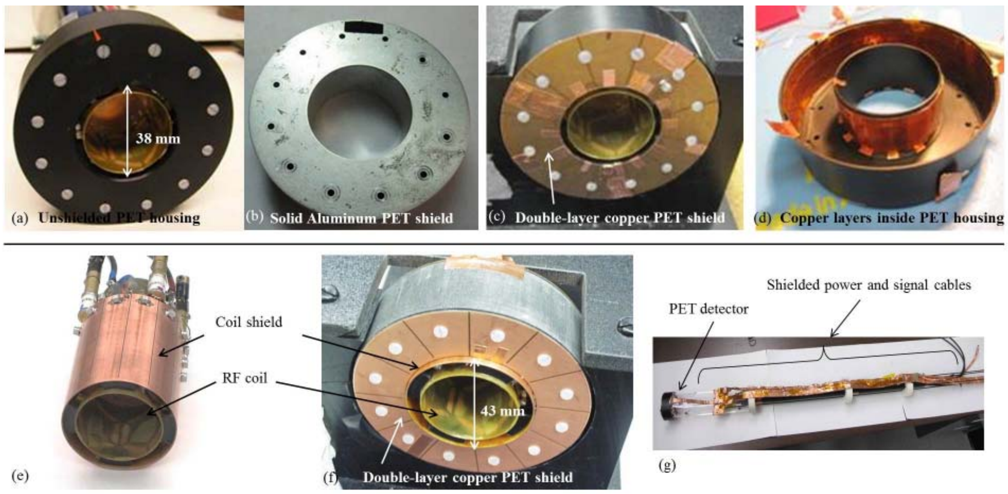
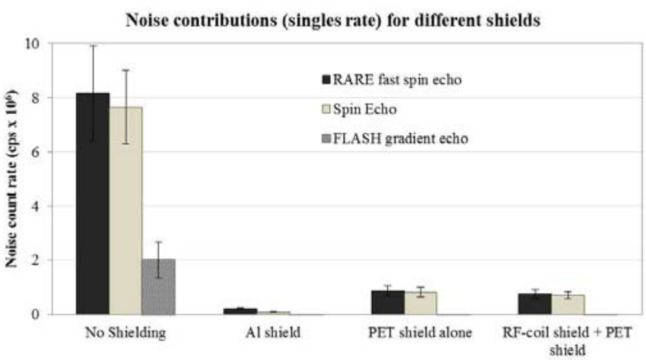


Figure 1. Various RF shield configurations built and tested.



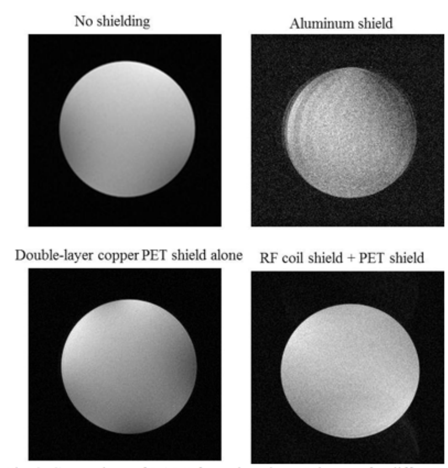


Fig. 8. Comparison of RARE fast spin-echo MR images for different shields.

Figure 2. Left: Effects on singles rate of the RARE, spin echo, and FLASH MRI pulse sequences on the different shield configurations. Right: Effects of different shielding configurations on MRI image quality.

PLANS:

We will return to the University of Pennsylvania to test how our latest electronics performs within their 9.4 T large-bore MRI. The funding has run out, but this work will likely continue, funded by SynchroPET, Inc. so that they can finalize our small-animal PET-MRI as a product and market it.

Estrogen Biosynthesis as a Novel Imaging Target with Multiple Applications

LDRD Project 11-051

Anat Biegon

PURPOSE:

The goal of the work pursued was to explore the availability and role of aromatase in different brain regions and peripheral organs in healthy subjects and use this new knowledge for the exploration of the use of aromatase in normal brain function as well as a diagnostic or treatment target in a wide spectrum of diseases.

APPROACH:

Steroid biosynthesis is a multistep process starting with the transport of cholesterol for the cytoplasm into mitochondria and ending with the aromatization of androgens to estrogens. The first, rate-limiting step, is mediated by peripheral benzodiazepine receptors (PBR) and the last step is uniquely catalyzed by aromatase (Cyp19a gene product). Estrogen is a pluripotent hormone involved in a large number of physiological processes, including, among others, the maintenance of reproductive function, bone density, sexual behavior and cognitive function. Estrogens also play a crucial role in several types of cancer and in obesity. Increased density of PBR is associated with tumor progression and inflammation caused by bacteria, viruses and autoimmune disease.

The relationship between regional brain aromatase, personality traits and normal brain function (e.g. verbal memory) and the effects of smoking were studied in collaboration with Dr. N. Alia-Klein from the Neuropsychology group. Studies on the involvement of brain aromatase in obesity are performed in collaboration with Dr. G.-J. Wang. Breast cancer studies are planned in collaboration with breast surgeons and radiologists from Stony Brook University (SBU) Medical School and the University of Pennsylvania. Protocol development in Alzheimer's disease involved collaborators from SBU Medical School's Department of Psychiatry, neuropsychology service and VA Hospital.

TECHNICAL PROGRESS AND RESULTS:

<u>Recruitment/scanning</u>: A cohort of overweight (BMI 26-30) and obese men and women (BMI>35, N=12) was scanned following the protocol approval (July 2012) and the results are undergoing analysis.

<u>Data analysis</u>: Results of brain and body scans of 30 healthy subjects were completed during this fiscal year. Kinetic modeling and analysis was completed for brain regions with high uptake (thalamus, amygdala). A simpler approach (calculation of standard uptake values, SUV) was taken for other brain regions and body organs where total tracer uptake was too low for complex modeling. Validation, distribution, pharmacokinetics and modeling of [11C]vorozole in healthy human brain was accomplished and published. Briefly, the regional distribution of [11C]vorozole in the human was found to be highly regional and unique. The highest concentrations of tracer were found in thalamic nuclei, followed by amygdala and inferior olive. As expected, tracer uptake was reduced following administration of a pharmacological dose of letrozole. Kinetic modeling of the blood and brain activity curves showed that a two tissue compartment model was superior to a single compartment model and equally suitable to the model-independent Logan graphic analysis.

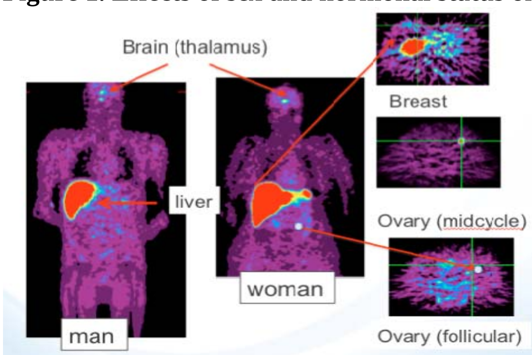
<u>Brain aromatase involvement in personality and cognition</u>: we found a significant, positive correlation between aromatase levels in amygdala and trait constraint, which was especially significant in women. Brain levels of aromatase were also correlated with verbal memory in a region- and sex-dependent fashion.

Brain aromatase involvement in obesity: Overweight and mildly obese women were found to have significantly lower levels of aromatase in several brain regions, with the largest effects found in amygdala and hypothamus.

Brain aromatase and cigarette smoking: Six smokers were scanned recruited (2 men and 4 women). Four (2 men and 2 women) had measureable amounts of nicotine and cotinine in the blood on the day of the study. These subjects had lower aromatase availability in the thalamus and amygdala compared to controls matched for age, sex and BMI. The 2 light smokers with no nicotine “on board” at the time of study were not different than non-smoking controls, supporting the theory that nicotine and cotinine block brain aromatase *in vivo* in a reversible manner.

Aromatase in peripheral organs: Tracer concentrations in most peripheral organs (heart, kidney, lungs, bone and muscle) were low and short lived, with several notable exceptions including the liver in all subjects and the ovary in young women imaged at midcycle (Fig. 1). Liver uptake was not blocked by letrozole, suggesting radioactivity in this organ reflects metabolism and/or tracer binding to another target, possibly another cytochrome p-450 linked enzyme (Fig. 1).

Figure 1. Effects of sex and hormonal status on [11C]vorozole uptake in the human body



	Count	Mean	Std. Dev.	Std. Err.
ef	3	1.287	.100	.058
ll	5	1.516	.407	.182
mc	8	5.029	2.985	1.055

	Mean Diff.	Crit. Diff.	P-Value	
ef, ll	-.229	3.475	.8888	
ef, mc	-3.742	3.221	.0261	S
ll, mc	-3.513	2.712	.0151	S

	DF	Sum of Squares	Mean Square	F-Value	P-Value	Lambda	Power
Period	2	51.903	25.951	5.351	.0202	10.702	.745
Residual	13	63.050	4.850				

Left: [11C]vorozole in male and female body. Right: One way ANOVA comparing ovarian SUVs in the early follicular (ef), late luteal (ll) and midcycle phases of the menstrual cycle. S=p<0.05, Fisher’s PLSD posthoc.

Effects of sex, age and hormonal environment: Aromatase levels expressed by SUV were higher in the male brain relative to the female brain (significant effect of sex, no sex x brain region interaction). SUVs declined with age throughout the brain in both men and women. The hormonal environment (stage of menstrual cycle, menopause) in women had a significant effect on SUVs in the ovary, where midcyle levels (high estrogen) were more than two fold higher than levels in the early follicular or late luteal stage. In the brain (e.g. amygdala) early follicular and midcycle levels were higher than those in the late luteal phase or after menopause.

Significance: The results summarized here indicate that [11C]vorozole is indeed a novel and useful tool for measuring aromatase availability in the living human brain and body. The data gathered from healthy subjects helps reveal the role of estrogen synthesis capacity in normal physiology and provide a baseline for future studies of various brain neuropathologies and brain cancer. The data gathered from peripheral organs provides a baseline for positron emission tomography studies of aromatase as a diagnostic and/or prognostic aid for cancers of peripheral organs and pathologies of the female reproductive system.

Plans: We plan to complete kinetic analysis of more brain regions and peripheral organs as outlined in the original submission and submit an Investigational New Drug (IND) application by the end of the grant period, followed by protocols and grant applications in specific areas including obesity and breast cancer.

High-Throughput Screening in Biological Systems Using Radiometric Approaches

LDRD Project 11-053

Richard A. Ferrieri

PURPOSE:

Our aim is to identify and develop potential technologies using short-lived radioisotopes in combination with non-invasive imaging and radiometric bioassays that not only support the general systems biology approach to conducting research in plant sciences but also are amenable to development into high-throughput screening tools for assessing gene function in systems relevant to the DOE mission to harness biomass feedstock for alternative renewable energy. Our emphasis in the last years has been to develop rapid *in vivo* imaging approaches for screening basic root functions in intact plants. These new tools offer potential for program growth aligned with the DOE Bioenergy Centers providing a needed National resource in screening new lines of genetically engineered feedstock and for assessing sustainability of future feedstock when grown under marginal conditions.

APPROACH:

Positron emission tomography (PET) imaging provides a unique look at the dynamic processes involved from the fixation of atmospheric CO_2 to its conversion to sugars and their transport belowground to roots where they are used in growth and storage. We have identified several basic plant functions including root allocation, transport speed and root exudation, and have been working this past year to define the relationship of these basic functions to root sink strength for carbohydrates and root growth rates. Root radiography also provides opportunities to capture snapshots in time of root allocation giving higher spatial resolution than PET and information on growth characteristics as a function of root system architecture including root branching.

TECHNICAL PROGRESS AND RESULTS:

Plant root physiology is an often-neglected part of basic plant function owing to the lack of investigational tools that enable one to measure root responses to environmental cues. Last year, we developed a root phenotype screen involving measuring shoot-root allocation, root transport speed and root exudation of ^{11}C-photosynthate using a combination of PET imaging, root radiography and nuclear counting in conjunction with administration of $^{11}CO_2$ to leaves of intact plants. From studies conducted by our group spanning across many grass models, we realize that general perceptions about plant roots and how they respond to environmental cues may be inaccurate due to the lack of direct experimental measurements of their physiological responses. For example, it seems intuitive that root sink strength for aboveground carbohydrates would be driven by the density of the root biomass. However, in our preliminary studies reported last year using Caiapo rice plants, we demonstrated that plants grown on high iron versus low iron exhibited an inverse correlation between root biomass and root sink strength for ^{11}C-photosynthate. We realize now that what these early studies lacked was a direct correlation between our radiometric physiological root assays and root growth rates to give biological relevance to our measurements. Experimentally, this is possible to measure non-invasively using PET imaging by retesting same plants over several days of growth. While PET root imaging does not afford opportunity to measure disposition of radiotracer with high spatial resolution, it does enable us to measure the movement of radiotracer through individual roots and determine changes in root length and in sink strength through transport and allocation of ^{11}C-photosynthate.

A key advantage of using a PET radioisotope like carbon-11 over other carbon isotopes is that its 20.4 minute radioactive half-life affords a unique opportunity to retest the same plant over time. We have recently enhanced our imaging capabilities through the acquisition of RootSnap (CID Biosciences, Inc.), a diagnostic root imaging system that enables measurement of root growth parameters using contrast digital photography, and have begun integrating its use with our PET root imaging protocols.

One of the major challenges we face is to increase throughput of whole-plant PET imaging using the HR+ scanner. Our original concept for multi-plant microPET imaging was demonstrated in 2011 for imaging up to six small grass plants simultaneously. To increase capacity would require use of the larger human HR+ scanner. The challenge here is the imaging cassette will be too large (~ 1m in diameter) to shield with lead for safe transport between the plant radiotracer laboratory and the imaging facility. To meet this challenge, we are presently refining technology that will enable us to build a miniaturized $^{11}CO_2$ pulsing cassette to safely transport high doses of ^{11}C-tracer to the imaging site for administration.

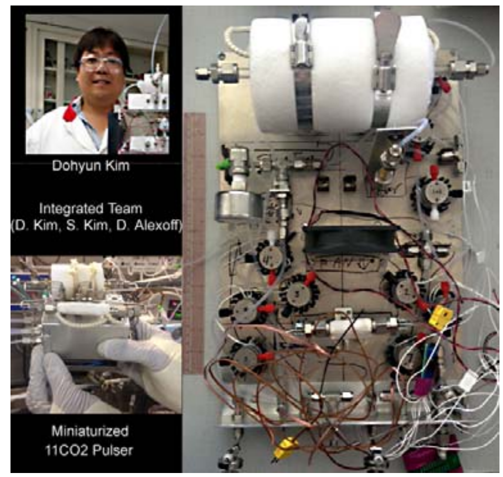


Figure 1. Our integrated team of engineers has successfully miniaturized our standard $^{11}CO_2$ pulsing station, seen on the right side, to a hand-held unit shown on the left side.

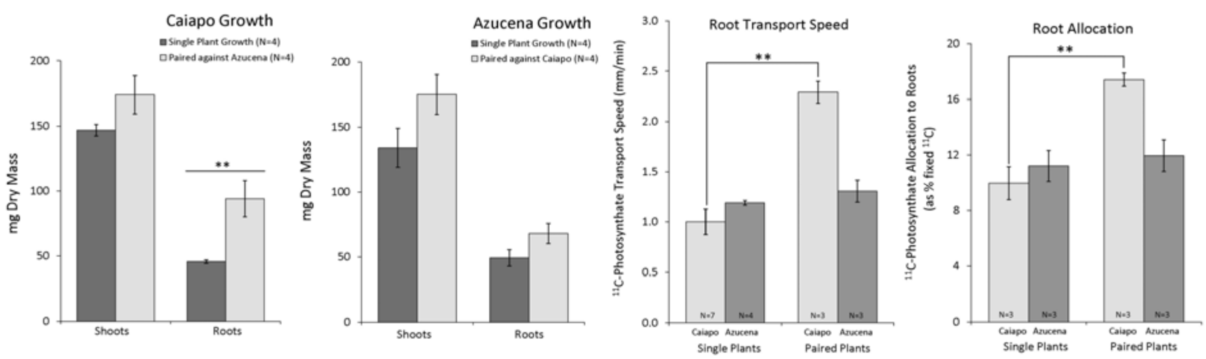


Figure 2. New insights into basic root functions revealed by PET imaging of competitive plant systems.

This year, we also continued to explore new biological applications for multi-plant PET imaging by examining basic root functions between rice genotypes, Caiapo and Azucena that were forced to compete with each other for limiting nutrients belowground when their root systems were allowed to overlap. This application has strong relevance to the DOE mission in bioenergy where bioenergy crops will likely be planted close

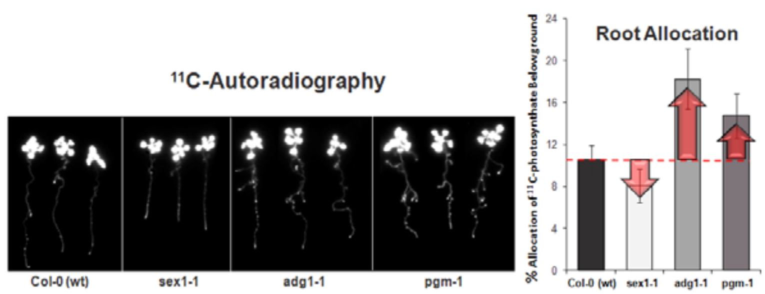


Figure 4. Screening 12 day old Arabidopsis seedling mutants with alteration in starch biosynthesis using ^{11}C-radiography gives opportunity to look at impact of plant carbohydrate metabolism on root growth. The starch abundant mutant (sex1-1) allocates less carbon to roots relative to wild-type (Col-0) resulting in slower root growth. The starch deficient mutants (adg1-1 and pgm-1) allocate more carbon to roots resulting in increased root growth and excessive lateral root patterning.

together on marginal soils that possess limited resources for growth. Plant competition for resources will no doubt be fierce amongst plants impacting their overall hardiness for sustainable growth. What we found in these early studies is Caiapo plants exhibited increased root growth when grown in close proximity (1 cm) to Azucena plants as compared to isolated growth. PET imaging revealed that ^{11}C-photosynthate was moving within Caiapo roots at higher transport rates and at higher relative amounts than in Azucena when plants were paired.

These findings were reported at the International Society of Root Research this past July.

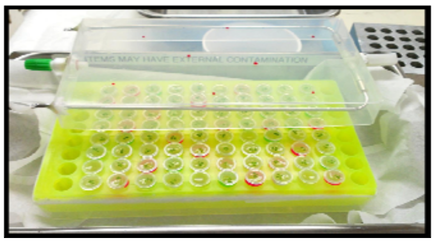


Figure 3. Array seedling chamber for simultaneous administration of $^{11}CO_2$ tracer.

We have also begun integrating root radiography into our higher throughput screening effort. Radiography affords an additional opportunity to capture a high resolution snapshots in time of the radiotracer distribution between the primary and branch root structures (i.e. lateral roots) giving feedback on how root system architecture impacts growth rate and overall root sink strength for non-structural carbohydrates. A goal of this effort is to establish a direct relationship between our radiometric root functions (including resource allocation both to primary and fine root structures, transport speed and root exudation) and root growth. We believe that root growth will be positively correlated with increases in these basic root functions. Furthermore, we believe that overall root density will not be a major driver defining root sink strength, but rather the root substructures (i.e. lateral root branching) and their growth rates will be the defining factor. Further detailed studies are needed that scale across other grasses in order to generalize the relationship between root function and root growth rates.

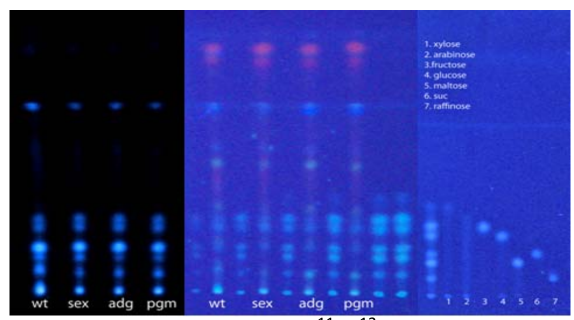


Figure 5. Visual assay of $^{11}C/^{12}C$ sugar profiles from plant tissue extracts using radio and fluorescent thin layer chromatography.

Finally, we have begun to apply many of the tools described above to screening hundreds of tiny seedlings for their ability to fix $^{11}CO_2$, metabolize the tracer into sugar pools and move those sugars to roots. In a pilot study using starch mutant seedlings from the *Arabidopsis* plant model we were successful at adapting our high throughput imaging for assessing root growth dynamics. Furthermore, we were successful at adapting high throughput visual radiometric bioassays for quantifying new and old carbon fluxes into non-structural carbohydrate pools. This is the only technology of its kind that can do

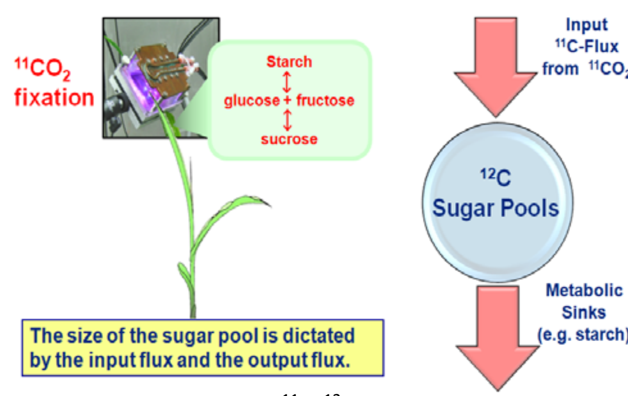


Figure 6. Flux assay of $^{11}C/^{12}C$ isotopic signatures in metabolite pools affords opportunity to assess the metabolic machinery of plants in response to environmental cues and/or molecular traits.

these measurements with this efficiency.

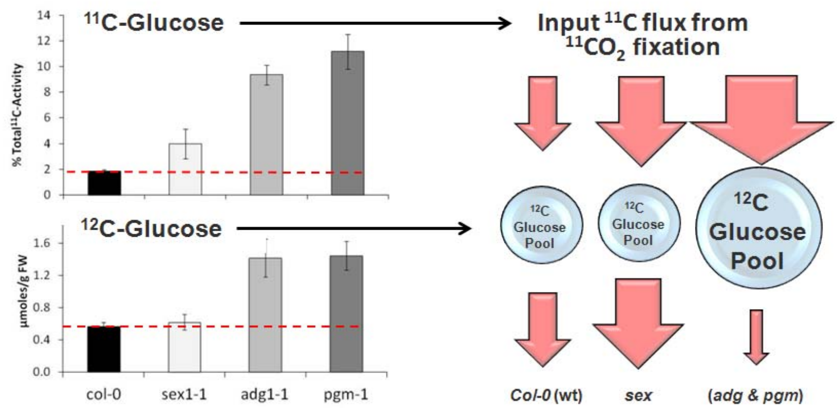


Figure 7. Starch mutants exhibit very different metabolic fluxes as demonstrated by this data showing changes in the glucose sugar pool.

Astrophysics and Cosmology Initiative

LDRD Project 11-055
Anže Slosar

PURPOSE:
The purpose of this LDRD was to kickstart cosmology research at BNL. In particular, we have tried to bring a method for mapping the high redshift universe through the Lyman-alpha forest to the level suitable for precision cosmology.

Approach:
Lyman-alpha forest is a set of absorption features, blueward of the Lyman-alpha emission feature in the spectra of distant quasars that correspond to the absorption by the intervening neutral hydrogen between the source and us. These can be used to make a one-dimensional map of the fluctuations in the hydrogen density along one particular line of sight. When many such quasars are combined, one can attempt to make a three-dimensional map.

BOSS experiment was the first for which the number density of quasars on the sky is sufficiently large to be used as a three-dimensional probe of the universe. Our goal was to use this technique to detect the baryon acoustic oscillations at high redshift.

TECHNICAL PROGRESS AND RESULTS:
In the early fiscal years we have worked in establishing the basic method as a valid method for measuring the three-dimensional structure of the Universe at high redshift. This has resulted in an important paper (Slosar et al, 2011) that has demonstrated the feasibility of the method and shown that theory is consistent with predictions for correlations up to 100 Mpc/h.

Since then we have attempted to detect Baryonic Acoustic Oscillations in the data. There were two semi-independent groups working on this detection. The basic datasets were the same and the mock data were provided by me and collaborators. This work resulted in 3 papers:

Busca et al (Slosar is in the 2nd of 3 tiers of authors): with the first detection, currently submitted to A&A: this paper provided the first detection of BAO in the Lyman-alpha forest at around 3-sigma level.

Slosar et al, currently in collaboration review: this paper provided a stronger detection of BAO with a more complicated method and arguably more careful treatment of systematics

Kirkby et al. (Slosar is second author): this paper provided a careful analysis of the BAO fitting techniques

In Slosar et all, we have measured the position of the BAO peak with a 2% statistical and 1% systematic errors. Our results are consistent with the standard LCDM cosmology.

The LDRD has now expired. The BOSS experiment has been very lucky with the weather and is likely to finish early (~Jan 2014). We hope to have better analysis ready by then.

PI is currently working on improved data analysis methods. We expect more papers to be coming in the next few years.

Complex Modeling for Nanostructures

LDRD Project 12-007

Simon J. L. Billinge and Pavol Juhas

PURPOSE:

The aim of this project is to develop data analysis methods and software for solving complex global optimization problems that combine multiple experimental and theoretical inputs. The project is focused on solving atomic structure of nanomaterials and other materials with nanoscale structural distortions. We plan to develop a software framework that can efficiently define complex modeling problems and solve them with powerful optimization methods. We will use the first-principles modeling experience and computing resources at the Computational Science Center at BNL. We have identified several scientific problems, intractable with the current data analysis techniques that should yield to our complex modeling approach. The examples include CdS-ZnS core-shell nanoparticles with tunable band gap, white light emitting ultra-small CdSe nanonparticles, stable nanoclusters of gold, and local stacking of organic molecules. Once successful, we expect a great response in the scientific community as well as considerable interest from the funding agencies to provide long term funding for these developments.

APPROACH:

Accurate determination of atomic arrangements in nanomaterials is often beyond the means of current structure analysis techniques. Conventional single-crystal or powder diffraction measurements provide few if any Bragg reflections, as there are not enough atoms to form periodic motifs in the material. TEM and SAS techniques can provide information about nanoparticle size and shape, but do not yield accurate atom positions. Atom positions can be well determined for nanoparticles that crystallize in a regular super-structure, but that is a very rare case. The atomic pair distribution function technique is very sensitive to atom arrangements at a local scale, but has lower accuracy for overall particle shape and for boundary features in a core-shell structure. The extended x-ray absorption fine structure (EXAFS) can distinguish specific pairs of atoms in the structure, but cannot probe lengths beyond first-few coordination spheres. Theoretical DFT simulations are computationally expensive and require approximations, which need to be experimentally verified. Most of the existing data-analysis software works with a single experimental or theoretical method, while the programs that combine several techniques together do so in a specialized non-flexible way. (EPSR) Nanostructures lack symmetry and require more information for their accurate characterization. At the same time, the experimental probes become less resolved and carry less signal when applied to nanomaterials. To address this situation, it is necessary to combine information from several experimental and theoretical sources in a single optimization problem, allowing the techniques to complement each other and achieve global minimum with reliable structure results. We plan to use the pair distribution function, SAS, EXAFS and possibly TEM techniques on the experimental side together with the known chemical constraints and first-principles theoretical simulations of materials.

TECHNICAL PROGRESS AND RESULTS:

The complex modeling effort is based on the existing Python and C++ codes developed in the Billinge-group as part of the diffraction sub-group within the NSF funded DANSE software project. The libraries cover PDF simulations for crystals and finite cluster, bond valence sum calculations, evaluation of atom radii overlap, bond angles and distances and the Liga algorithm for a smart build-up of trial structures. The code was designed with object-oriented paradigm allowing for extensions and tweaks for specialized structure simulations. As an example, the software can be easily enhanced with a custom PDF profile functions or user-defined peak broadening model that reflects vibration modes in the material. The SrFit library is a crucial high-level component that wraps PDF modeling, SAS simulations, constraints and restraints in a single optimization problem. The software was applied for a simulation of experimental PDFs measured from several crystalline phases of quinacridone. These systems contain rigid quinacridone molecules arranged in layers and their experimental PDFs contain sharp features from a single molecule as well as broad features from inter-molecular correlations. We have used simulations with separate single-molecule and crystal PDF contributions, which let us study the stacking and vibrations of quinacridone molecules. We have also studied 144-atom gold nanoparticles, where the PDF measurements showed discrepancy with the established minimum-energy structure. The experimental PDF could be better simulated as a combination of HCP and FCC spherical shape cutouts pointing at close packed arrangement of atoms in the nanoparticle. We have developed a cluster buildup routine that creates close packed test structures and are working with Dr. Yan Li at the BNL Computational Science Center to screen them for optimum energies and for match with the experimental PDF. We are working on speed optimization of our codes and on their deployment on the BNL BlueGene supercomputer.

Milestones:

YEAR 2

- Implement RMC-style global optimizer, reproduce one of the established RMC examples with our code. Work towards more robust big-box modeling than current RMC methods
- Implement fast updates in the PDF calculator, i.e., recalculate contributions for a single atom if only one atom position changed.
- Solve Au or CdSe NP using the CM approach
- Publish papers that describe the srreal and srfit frameworks
- Implement Parametric PDF refinements that complex multiple datasets that have been measured as a function of variations in some external parameter like temperature.
- Get framework working on BNL high performance computing resources and make a complex that includes theoretical molecular modeling or ab initio calculations
- Make first attempts at using Uncertainty Quantification applied to the nanostructure inverse problem

YEAR 3

- Use year 2 results to make a compelling proposal for a large SciDac or similar grant to take on robust modeling based on the complex modeling paradigm
- Begin integrate of our codes with NSLS-II data-streams and work on making them more accessible to the user community.

Early Deployment Flagship Applications on BG-Q

LDRD Project 12-008

Michael McGuigan and Yan Li

In this report we document the progress on the deployment of applications in the three areas covered by the research: complex modeling of nanostructures, development and deployment of scalable codes for accelerator physics, and lattice QCD.

Complex Modelling for Nanostructures (*Yan Li*)

PURPOSE:
This project is in collaboration between the Computational Science Center (CSC) and Dr. Simon Billinge's group in the Condensed Matter Physics and Materials Science Department to demonstrate the use of complex modeling scheme for solving the structure and properties of nanostructure. The goal is to develop and demonstrate some parts of the global optimizer scheme Billinge proposed, in particular, the pair-distribution-function (PDF)/theory & modeling complex.

APPROACH:
We have applied advanced first-principles computational tools to a series of nanostructures (for example, bare and ligand-protected Au clusters, CdSe quantum dots etc) to determine their atomic structures and to probe into their physical properties such as energetic stability, energy gap and optical properties. Both density functional theory (DFT) and DFT-based tight-binding methods have been employed and calculations were carried out using mainly the VASP package (DFT) and the dftb+ (DFTB) package. Highly parallel quantum mechanical calculations utilizing up to 10^2-10^3 processors are being tested on the Blue Gene/Q machines at BNL.

TECHNICAL PROGRESS AND RESULTS:
During FY 2012, we have carried out the following tasks. With the assistance of CSC staff Len Slatest, we have ported a suite of quantum-mechanical simulation code from BG/L and P to BG/Q, including VASP, Quantum-espresso, abinit and Qbox etc. Extensive parallel tests are currently being carried out. We have performed scaling tests using VASP on BG/Q and compared its performance on BG/L and BG/P. To develop, test and demonstrate the PDF/theory complex of the global optimizer scheme, we have studied two systems at the first stage: the gold nanoparticle Au_{144} terminated with 60 thiolates, and ligand-protected $Cd_{35}Se_{28}$ cluster, both of which have been characterized by X-ray diffraction by Billinge's group.

Development and Deployment of Scalable Codes for Accelerator Simulation (*Roman Samulyak*)

PURPOSE:
The goal of this project is the development and deployment of highly scalable codes for the simulation of processes in particle accelerators. Our project has two main objectives: the development of particle-based hydro- and magnetohydrodynamic (MHD) code in the low magnetic Reynolds number approximation (weakly conducting media) for multiphase systems and its application for the simulation of liquid mercury jet targets for the DOE Muon Accelerator Project (MAP). The other objective is the development of an advanced electromagnetic Particle-in-Cell (PIC) code for the simulation of processes relevant to e-RHIC and advanced acceleration methods.

APPROACH:
The multiphase MHD code is based on our novel Lagrangian particle algorithm that extends and improves ideas of smooth particle hydrodynamics and on advanced programming methods that parallelize the code for both traditional and Graphic Processor Unit (GPU) supercomputers. The electromagnetic PIC code is based on scalable symplectic integrators for particles and fields optimized for multicore supercomputers.

TECHNICAL PROGRESS AND RESULTS:
During the first year of the project, new Lagrangian particle MHD code has been developed for traditional and GPU supercomputers. The code is being used to provide simulation support for the DOE MAP project. The deformation of the mercury jet target in strong magnetic fields and the interaction of the target with high-energy proton pulses have been calculated. These studies contribute to the target design for the future muon collider. The electromagnetic PIC code has been developed and optimized on multicore supercomputers. The code is being used for the study of processes relevant to the future e-RHIC facility at BNL and processes relevant to the muon cooling within the MAP project.

Lattice QCD

Chulwoo Jung, Frithjof Karsch, Taku Izubuchi, Hyung-Jin Kim

PURPOSE:
To efficiently utilize the new state-of-the-arts computing resources, including IBM BlueGene / Q and Graphic Processor Unit (GPU), for Lattice QCD we aim to develop and port in-house QCD libraries as well as software developed by the lattice QCD consortium USQCD. Furthermore, we examine and develop new algorithms for more efficient lattice QCD computing.

APPROACH:
Having the enormous progress of hardware, especially IBM BlueGene/Q and GPUs, the lattice QCD softwares needs to be developed and/or ported to run efficiently on these new environments. There are particular parts of lattice QCD computing that need to be developed for the new resources: the kernel code to describe interaction of quarks (Dirac operators), calculation of the gluon interaction in the Molecular Dynamics Efficient solver for the equations of motion of quarks using low modes of the Dirac operator, finally to demonstrate new physics computation that can't be done in previous computing resources and software.

TECHNICAL PROGRESS AND RESULTS:
For BG/the efficient Dirac operator for domain-wall lattice quark, and gauge force term has been implemented, and ported into the Columbia Physics QCD library (CPS++). It now achieves around 30% of the theoretical peak speed with excellent scalability. This code is now in production for the QCD vacuum ensemble generation for physical light quark on big (~5fm) lattice for zero and finite temperature. The code is also used on BG/Qs at Argonne National Lab, Lawrence Livermore National Lab, and University of Edinburgh. Dr. Kim is also looking into the optimization of various code necessary for calculating physical quantities such as Kaon Bag parameter on BG/Q. Kim has been working on lattice QCD computation crucial for muon's anomalous magnetic moment, g-2, for which a new large scale experiment is planned at Fermi Lab. The new ideas for the hadronic vacuum polarization contribution, with techniques of reducing statistical noise with the low mode of Dirac operators, are being examined.

Inter-individual Variation in Radiation Induced Epigenetics

LDRD Project 12-012

Paul F. Wilson

PURPOSE AND APPROACH: The goal of this project is to understand the impact of DNA and protein-based epigenetic modifications on cellular radiation responses following accelerated proton and HZE ion exposures delivered at the NASA Space Radiation Laboratory (NSRL), specifically to shed insight on the roles of these regulatory pathways in modulating DNA double-strand break repair, chromosomal aberration induction, cell survival, and ultimately radiation carcinogenesis. Two primary research questions will be addressed in these experiments. First, do proton or heavy ion exposures result in the induction of 5-hydroxymethylcytosine (5-hmC) via radiochemical conversion of 5-methylcytosine (5-mC) as we see for low LET gamma irradiation, and does 5-hmC induction affect gene expression at key radiation response loci? Second, does treatment of human normal and tumor cells with clinical histone deacetylase (HDAC) inhibitors (currently used as chemotherapy agents) prior to proton/HZE ion irradiation result in enhanced radiosensitization as we observe for low LET gamma irradiation? This second major aim will produce a comprehensive set of survival data for the relative effectiveness of other HZE ions besides protons or carbon (i.e., helium or oxygen) for killing tumor cells derived from the sites currently treated with protons or carbon ions due to their intrinsic radioresistance or proximity to radiation-sensitive tissues/anatomical structures. This project will provide information as to whether these DNA and protein-based epigenetic modifications result in increased levels of DNA damage, impairment of DNA repair capacity, increased cell killing and IR-induced cellular transformation using an established surrogate *in vitro* tumorigenesis assay of anchorage-independent growth in soft agar.

TECHNICAL PROGRESS AND RESULTS: The following is a brief summary of our results for FY2012.

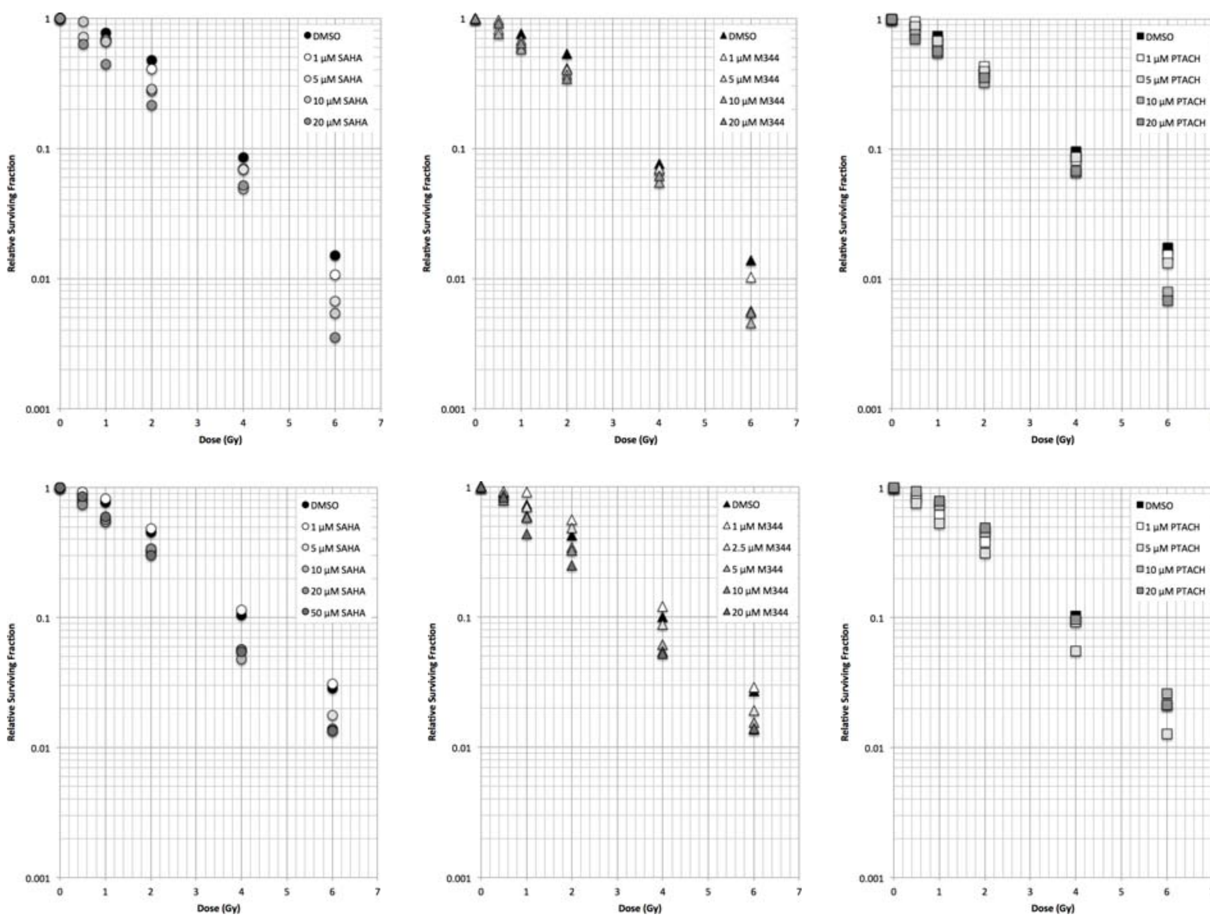


Figure 1 (previous page). Gamma ray survival curves of U2OS osteosarcoma cells (top panels) and NFF28 normal human fibroblasts (bottom panels) treated with HDAC inhibitors SAHA/Vorinostat (left panels), M344 (center panels) or PTACH (right panels). These experiments are needed to determine maximal concentrations of HDAC inhibitor, plus serve as the low linear energy transfer (LET) controls for proton/heavy ion irradiations at NSRL. U2OS osteosarcoma cells are more radiosensitive than NFF28 fibroblasts (both are mesenchymal-derived cell types), plus a greater degree of HDAC inhibitor radiosensitization was observed for U2OS compared to NFF28. Curiously, only 5 µM PTACH in NFF28 fibroblasts resulted in radiosensitization, while the remaining concentrations had no effect; NFF28 survival with 1 µM M344 or PTACH is increased relative to DMSO (drug vehicle) control. We have achieved highly consistent results over 1 year of experiments (with dozens of experiments conducted), giving us confidence to move to the NSRL irradiations of these lines in FY2013.

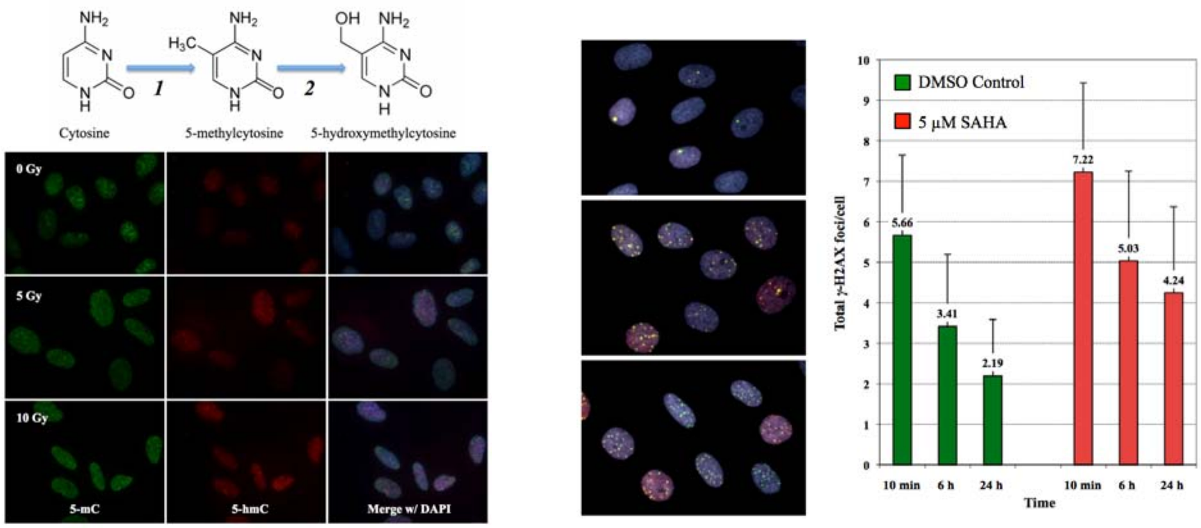


Figure 2. Left top panel: Conversion of cytosine to 5-mC is accomplished by DNMT-mediated transfer of a methyl group to the C5 position (step 1); and its subsequent conversion to 5-hmC is accomplished by TET protein-mediated transfer of a hydroxyl group or via oxidative radiochemistry. Left bottom panel: Immunocytochemical detection of 5-mC and 5-hmC in NFF28 human fibroblasts using antibodies specific to 5-mC and 5-hmC (Active Motif) demonstrating IR induction of 5-hmC. Right panel: Gamma-H2AX DSB foci levels in G0/G1-phase cultures treated with 5 µM SAHA or DMSO control and irradiated with 25 cGy of cesium-137 gamma-rays. SAHA treatment results in ~2-fold higher baseline (sham-irradiated) levels of foci (0.79 for DMSO control; 1.66 for SAHA-treated), as well as slower kinetics of foci dissolution and 60% higher levels of unresolved foci 24 h post-irradiation. These ratios directly correlate with the higher dose cell survival assays above.

For the first year of this LDRD, we have had many scientific successes. These are in large part due to the efforts of my lab technician Alicia Johnson, former postdoc Dr. Pankaj Chaudhary (who left BNL in April 2012 for position in Ireland), and former co-investigator Dr. Krassi Botcheva (who left BNL in September 2012 for LBNL). In addition to the data presented in the above figures, Dr. Deborah Keszenman and Ms. Paula Bennett in my lab have developed a novel 5-mC/5-hmC-specific gel electrophoresis detection system using a modified Sutherland laboratory clustered DNA lesion detection assay and 5-mC/5-hmC slot blot detection using methylcytosine-specific antibodies. Several FY2013 publications are currently being prepared detailing these results, as well as proposals to NASA and NIH.

FY2013 Experimental Plan

- Complete NFF28, U2OS, and U87 glioma HDAC inhibitor gamma survival, foci, chromosomal aberration experiments; initiate gamma ray studies with remaining tumor cell lines (A549 lung carcinoma cells, HepG2 hepatocellular carcinoma cells, DU145 prostate carcinoma cells).
- NSRL irradiations of NFF28, U2OS, U87-MG, and V79 cells with protons, He, C, and O ions with lowest HDAC inhibitor concentrations required that achieve maximal radiosensitization.
- Analyze cell samples for 5-hmC induction ± HDAC inhibitors via immunocytochemistry and genomic analyses (5-hmC gel electrophoresis, 5-hmC-based loci-specific RT-PCR, ChIP-SEQ).
- Hire new postdoctoral fellow (position 16247 currently posted on BNL jobs website).

FY2014 Experimental Plan

- NSRL irradiations of A549, HepG2, and DU145 cells as described above. Prepare publications.

Developing an Integrated Atmosphere-Ecosystem Model for Investigating Interactions Between Atmospheric System and Ecosystem Under a Warming Climate

LDRD Project 12-015

Wei Wu and Alistair Rogers

PURPOSE:

The goal is to develop an integrated model for investigating the interactions (feedbacks) between the atmosphere and terrestrial ecosystems under a warming climate. As the Earth's surface temperature and atmospheric CO2 concentration increase, the Earth's surface and atmospheric energy flux (i.e., radiation fluxes, latent and sensible heat fluxes) and moisture fluxes will change. This change can lead to a change in cloud properties (e.g., cloud amount or optical depth) and rainfall pattern, and thus influences ecosystem properties such as photosynthesis and stomatal conductance. However, how the coupled atmosphere-ecosystem responds to a warming climate is still poorly understood. This project is aimed at filling in the blanks in climate studies by advancing our understanding of the interactions (feedbacks) between the atmosphere and terrestrial ecosystems as the Earth's surface temperature and atmospheric CO2 concentration increase. This project can also bridge the gap between climate and ecosystem studies by developing an integrated coupled atmosphere-ecological system as an effective tool. The success of this work can help advance the capability for climate prediction and broaden our horizons on climate-ecosystem modeling, and give BNL a significant edge in competing for funding in ongoing and future programs such as Atmospheric System Research or Earth System Modeling.

APPROACH:

The Earth's climate has been getting warmer since the last century, with increased global mean surface temperature [0.6°C ± 0.2°C from 1901 to 2000], melting of glaciers, and rising of sea level (IPCC, 2007). This warming trend is believed to be mainly induced by increased greenhouse gases (CO_2, CH_4 and N_2O) emissions from human activities such as burning fossil fuels and deforestation, and to have a significant impact on environment and natural resources including ecosystems and water resources. Understanding and predicting climate change and its interactions with ecosystems and water resources has thus been a major focus area of DOE mission priorities and BNL mission priorities.

The investigations proposed include: 1) the impact of land-surface properties (e.g., albedo and vegetation conditions) on the partitioning of atmospheric radiation fluxes; 2) the impact of soil moisture and vegetation on convection and severe weather under the current climate and a warming climate; 3) the impact of surface warming on the interaction between land-surface processes and atmospheric cloud-radiation processes; 4) the processes important for linking ecological system to the atmosphere, and their optimal parameterization; 5) climate feedback and uncertainty linked to atmosphere-ecosystem coupling.

The methods used include: i) use and improvement of the coupled Weather Research and Forecast (WRF) and Community Land Model (CLM); ii) use and development of radiative-transfer models; iii) use and development of single-column models from the BNL's FASTER testbeds; iv) develop a conceptual coupled 1-D atmosphere-ecosystem model; 5) use of existing ground- and satellite- based observations; 6) use of statistical methods for model-observation comparisons.

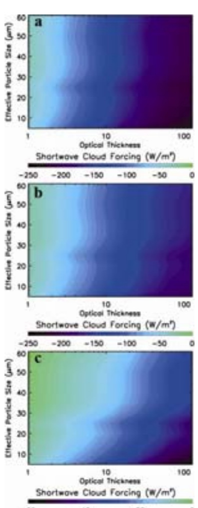
The current collaborators are: Thomas W. Collow (Ph.D. student), Mark A. Miller (Professor) and Alan Robock (Professor) at Rutgers University. Future collaborators are: Satoshi Endo (Scientific Associate II) and Wuyin Lin (Associate Scientist) at the BNL.

TECHNICAL PROGRESS AND RESULTS:

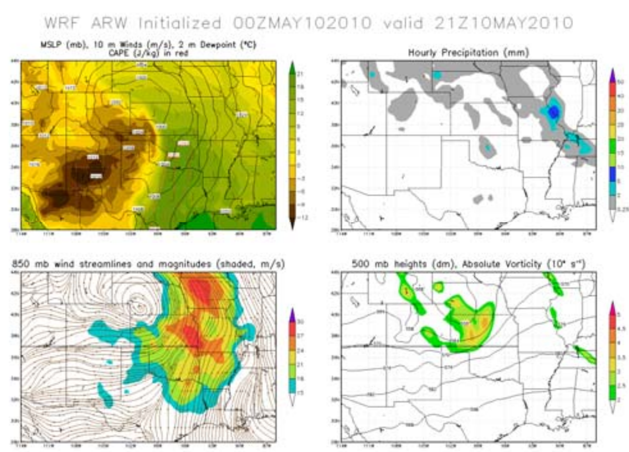
1) (By current postdoc at the BNL, starting from April 2012): tested the impact of land-surface albedo on modeling atmospheric radiation fluxes, by using two radiative-transfer models and a single-column model. We found that land surface albedo has a significant impact on modeling atmospheric radiation fluxes. For example, Figure 1 shows the strong dependence of the top-of-atmosphere shortwave cloud forcings on different land surface types (a: unfrozen lake and wetland with albedo 0.05, b: soil with albedo 0.2, and c: snow/dust with albedo 0.8)

2) (By current collaborators at Rutgers University, starting from Nov 2012): tested the WRF model's capability of modeling a significant severe weather outbreak. We found that the WRF is capable of modeling the environment for a significant severe weather outbreak. For example, Figure 2 shows the synoptic set up for the severe weather outbreak that occurred from May 10, 2010 to May 11, 2010 over the Southern Great Plains, Oklahoma. Upper left: the dewpoint which is shaded making the dryline across western Oklahoma and Kansas easily visible. An area of low pressure is also seen moving along the Kansas/Nebraska border. Upper right: precipitation just beginning to develop over Oklahoma. Lower panels: a strong low level jet emerging from the Gulf of Mexico at 850 mb (left) and a trough digging through the region at 500 mb (right).

3) (By Co-PI Alistair Rogers): examined the representation of photosynthetic CO_2 uptake in land-surface models, by comparing 12 models in parameterizing the maximum rate of carboxylation by the enzyme Rubisco ($V_{c,max}$). The value of $V_{c,max}$ is found to vary significantly in different models representing the same biomes. Thus, further improvement in estimating $V_{c,max}$ is highly suggested.



(Figure 1)



(Figure 2)

Milestones for each year of anticipated funding:

1) 2013: to complete and submit 1-2 papers; to investigate the impact of surface warming on the interactions between the Earth's surface energy and moisture fluxes and ecosystem processes;

2) 2014: to complete and submit 1-2 papers; to study the impact of the warming climate on the interactions between atmospheric cloud-radiation processes and ecological processes through land-surface energy and moisture fluxes.

Conical Slit for Probing Buried Micron or Sub-Micron Volumes for Dynamic Measurements of Heterogeneous Materials

LDRD Project 12-018

Ray Conley, Eric Dooryhee, Nathalie Bouet, Sanjit Ghose

PURPOSE:

Depth resolution in diffraction experiments is traditionally provided by a cross-beam technique with insertion of slits or pinholes in both the incoming and diffracted beam. This LDRD intends to implement a conical slit, with openings along the diffracting cones of the sample, to be fabricated with unprecedented accuracy using deposition and etching processes which will allow for submicron precision rather than electro-spark cutting which is limited to accuracies in the 5 to 10 micron range (allowing a minimum slit opening of 20-25 microns). The scope of the project is the design, deposition, and etching of the slits followed by a holder design that allows the 5 degrees of freedom necessary to properly align the slit. Experiments on proof of principle and a scientific study in the area of energy materials (particularly Solid-Oxide Fuel Cells) will be performed. A successful LDRD project will likely open this technique into a new area of research at NSLS-II, as well as at other synchrotron facilities around the world.

APPROACH:

The Conical Slit is an optical element first developed at RisØ National Laboratory, Denmark. It comprises of a set of conical openings positioned in accordance with the Debye-Scherrer rings of the phase to be investigated. Diffracted rays will be transmitted through the slit if and only if they originate from a three-dimensional gauge volume, defined by the beam size and slit opening size.

Historically, the intention was to generate three dimensional grain maps by scanning the slit or sample in the x, y, and z directions. The limitation on the gauge volume resolution was due to manufacturing issues. Wire electro-discharge machining of high Z metals (W) was used to fabricate the slits. Such a process could not create features below 20 microns in size. The recent fast paced progress made in deposition and chemical etching techniques both at BNL and other facilities has come to the point where a useful conical slit could be fabricated with this method allowing slit openings of 1 micron or less to be fabricated. By pushing the fabrication technology to a state of the art aspect ratio (> 5:1) and stacking 2 slits, the absorption of diffracted X-rays originating from outside the gauge volume by the slit can easily reach 99% using Pt.

The conical slit will enable 3D mapping of the strain tensor, crystallographic orientation, and structural refinement of all grains or sub grains in the defined volume, or the average within the volume, for highly deformed or extremely fine-grained samples (<20nm). In-situ experiments are possible as a function of temperature, strain, or field to follow dynamic processes. A proof of principle experiment will be performed which should lead to an instrumental paper; in the second year a focused science experiment on Solid Oxide Fuel Cells will be performed. Since the functional properties of these materials (and many other classes of energy storage materials) is strongly influenced by the local nanostructure at the electrolyte/electrode interface, an in-situ study following the buried 3D local dynamics at a micron to sub-micron length scale could dramatically increase the understanding of processes that occur during cycling. In particular, mapping the changes in composition, crystallography, and strain state at interfaces and triple phase boundaries could help correlate local nanostructure to properties, leading to new insights in the processing of this strategically important class of materials.

At the later stages of this project we hope to explore the production of spiral slits so that they may enjoy the substantial resolution increase of their conical predecessors.

TECHNICAL PROGRESS AND RESULTS:

The original LDRD proposal was drafted in FY11, and awarded to begin in FY12. Unfortunately, the original PI for this project executed no advancements or action towards this project. When the term for the original PI was not renewed at the lab, control of the project was transferred to the new team in approximately July of 2012. Immediately, a position description for the hiring of a Postdoctoral Research Associate was drafted and posted. The interview selection committee selected John Sinsheimer in the fall of 2012 to fill this position. At the time, John was finishing his last semester at Stony Brook University and completed his Ph.D. defense on December 17th. BNL made clear an intention to offer the position to John, however laboratory policy dictated that an official offer could not be made until after the successful completion of his defense. John officially reported to work on Monday, January 07, 2013.

Milestones for FY13 are as follows:
-Completion of two beamtimes related to x-ray powder diffraction at NSLS
-Ray tracing of the XPD beamline at NSLS-II leading to an appropriate slit geometry
-Proposal acceptance for slit fabrication at the CFN

Milestones for FY14 are as follows:
-Successful fabrication of a conical slit appropriate for use at an existing synchrotron radiation facility
-A science case demonstration utilizing the slit at an existing synchrotron radiation facility

In-situ Transmission X-ray Microscope Studies of Structure and Function in Energy Storage

LDRD Project 12-021

Jun Wang

PURPOSE:

Lithium-ion batteries are based on the principle of intercalation of lithium ions in host materials, both at the anode and at the cathode. All these materials, when subjected to the insertion and removal of lithium ions, undergo structural changes with range from minor changes in cell parameters to fully-fledged phase transitions or even materials' pulverization. Understanding the dynamics of these deformation processes can provide valuable information for establishing viable high-energy and high-safety batteries. The goal of this project is to in-situ monitor the electrode materials' behaviors (fundamental electrode reaction kinetics, microstructural evolution, and safety issues) within a working Li-ion battery by using Transmission X-ray Microscopy technique located at beamline X8C (National Synchrotron Light Source). The innovative research will substantially enhance our understanding of the fundamental mechanisms and stability of battery materials, and promote the development of advanced batteries techniques in transportation applications. This project also directly supports the key BNL mission of national energy research. Importantly, this research will develop new in situ techniques for energy studies, which will position BNL at a new frontier of energy research.

APPROACH:

Transition metals (oxides) are very promising candidates to replace used commercial battery material (graphite) due to their high capacities. However, these materials are subject to significant volumetric expansion and contraction during electrochemical reactions, which cause fast performance fading, structure instability, and safety problems. This LDRD project will employ TXM technique along with in-situ electrochemistry study to observe and understand the interior microstructure evolution of these battery materials. This technique has unique integrated advantages including deep penetration, chemical and elemental sensitivity, non-destructive and environmental free. Combing with x-ray absorption near edge structure (XANES) technique, in-situ 2D chemical and 3D tomographic imaging will proceed to study the electrochemical reaction, electronic structure and material degradation mechanisms. Synchrotron X-ray diffraction at Beamline 14A will further provide the crystal structure and phase transformation information of battery materials. Some conventional material study tools including SEM, TEM, and FIB will be used to prepare, observe, and study the experimental sample to supply further information for TXM work. This multidisciplinary approach will lead to a key evolution-property-performance correlation for these battery materials in Li-ion battery systems.

TECHNICAL PROGRESS AND RESULTS:

Considering the experimental requirement of TXM facility, it is challenging to design a functional battery to be compatible to the requirements to in-situ 2D and 3D experiment. It is a key for the success of this project. As to 2D insitu TXM study, we successfully designed and developed coin cells with Kapton windows which allow X-ray goes through the working battery, and performed the in-situ electrochemistry test (cyclic voltammogram) and tracked the morphology evolution via TXM image technique (in situ 2D study) at CuO materials (Fig. 1). For the first time, we combined the in-situ TXM imaging with XANES analyzing to provide detailed chemical and electronic structure information within the morphology evolutions during batteries cycling. With the supplemental information obtained from TEM, synchrotron XRD analysis, the electrochemical reaction mechanism and material degradation evolution were well understood. For 3D in-situ TXM study, we designed and assembled several microsized functional cells, and performed some basic in-situ electrochemistry studies. Although some challenges still remain, we obtained valuable experience on battery designs, 3D TXM studies, and electrochemical analysis. One of difficulties is material's stabilization at the designed electrode. We are developing new strategies including using FIB technique and novel carbon based porous electrodes.

This LDRD project started in June 2012.

Milestones (FY2013)
Q1: 2D TXM study of two lithium lithiation/delithiation mechanisms within battery materials (conversion reaction and alloy/dealloy reaction); Designing micro-sized functional cells for 3D study.
Q2: modify the cell's design and perform in-situ TXM 3D study on Sn based anode materials.
Q3: perform in-situ TXM 3D studies on other transition metal anode materials.
Q4: Correlate the morphology evolution to electrochemical performance/stability, and have new strategies to relieve the volume change such as applying carbon coating or alloying methods.

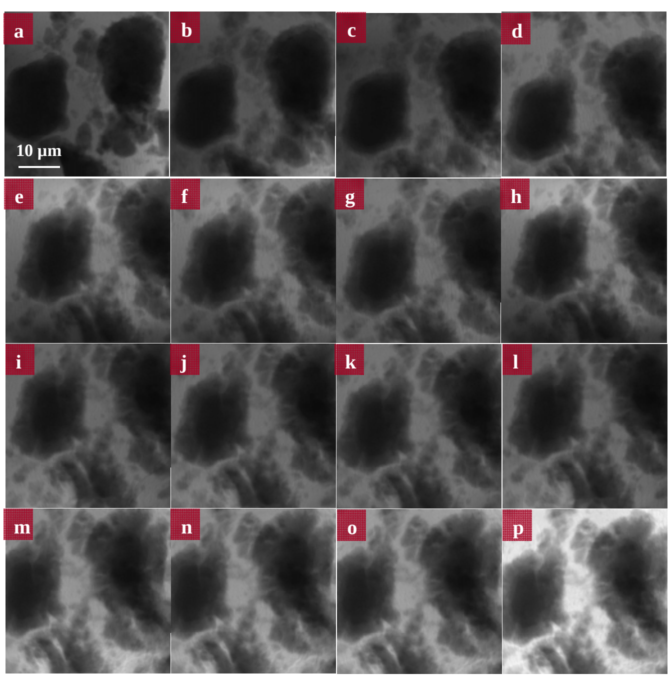


Fig. 1. In -situ TXM images of CuO particles within a real lithium-ion battery during operation.

MeV-UED for Ultrafast Science

LDRD 12-022

X.J. Wang, J.P. Hill & Yimei Zhu

PURPOSE:

We proposed the concept of MeV Ultrafast Electron diffraction (UED) based on a photocathode RF gun almost a decade ago [1], the objective of the current LDRD is to develop a MeV UED at BNL with the capable of producing the diffraction quality required to address the most important ultrafast scientific issues. We experimentally demonstrated high quality diffraction from a polycrystalline Al film with ~ 100 fs time resolution. The stringent test for any MeV-UED ever performed is the observation of super-lattice of a strongly correlated material, the visibility of super-lattice shows we have achieved signal to noise ration (SNR) better than 10^3. The success the LDRD lays the solid foundation for a future ultrafast science program at BNL.

APPROACH:

X-ray Free Electron Laser (XFEL) and Ultrafast Electron diffraction (UED) are two most important tools for exploring the ultra-fast and ultra-small world. UED has the advantages of large interaction cross-section and compactness; and DC gun based UED system has been successfully used to investigate structure dynamics from diluted samples (gas & liquid) to the strongly correlated material. The relative low beam energy (~ 100 KeV) limits the time resolution of the DC UED to ~250 fs. To reach the 100 fs time-resolution, we pioneered the idea of MeV-UED using a photocathode RF gun [1]. Higher electric field on the cathode of a RF gun makes it feasible to extract more electrons within a shorter bunch; and higher electron beam energy (MeV) will preserve the femto-second electron beam and eliminate the velocity mis-match between the pump and probe.

Taking advantage of the time-dependent electric field, bunch compression inside the RF gun could also lead to even shorter electron beam. One of the major challenges in realizing the MeV-UED potential is whether MeV-UED is capable of producing the diffraction quality required to address the most important ultrafast scientific issues. Other issue facing MeV-UED is the timing-jitter between the electron beam and pump laser. The mission of the BNL MeV-UED is to demonstrate high-quality electron diffraction with a sub-100 fs time resolution, and to develop a world-class ultrafast science program, particularly on the strongly correlated electron systems and transient structural dynamics. This LDRD is the collaborative effort between the BNL Photon Science and Basic Energy Science. Collaborators from China Shanghai Jiao Tong University and Florida State University also made significant contribution.

TECHNICAL PROGRESS AND RESULTS:

After successfully commissioned BNL MeV UED setup, the first sample used for our MeV-UED experiment is a polycrystalline aluminum. Fig. 1 is the single to 100 shots diffraction patterns of the 100-nm aluminum film, the number of electrons for each shot is about 10^4. The sensitivity demonstrated here is about 3 orders of magnitude higher than DC gun.

High-quality diffraction from a gold single crystalline is also obtained. The stringent test for the MeV-UED we have performed is the observation of super-lattice of a strongly correlated material. To realize the super-lattice, a series of improvements for our MeV-UED set-up were implanted in FY 2012. First, improvement in the brightness of the electron beam is critical. The single-shot diffraction capability of the MeV-UED is explored in real time - using the diffraction quality to optimize the laser and RF parameters. Dark current reduction and improving the diffraction detector sensitivity are also play important roles. The sample we used is TaS_2, Fig. 2 are the diffraction patterns of TaS_2. Fig.2 show we have experimentally demonstrated SNR is better than 10^3.

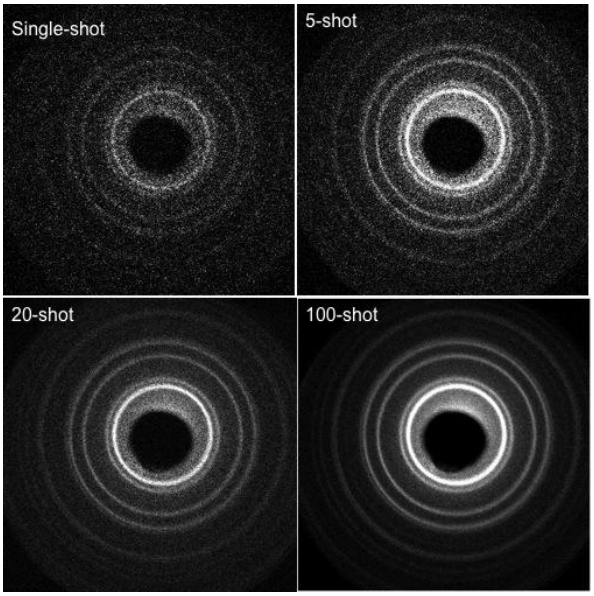


Figure 1: 100 nm aluminum film diffractions for single-shot to 100 shots.

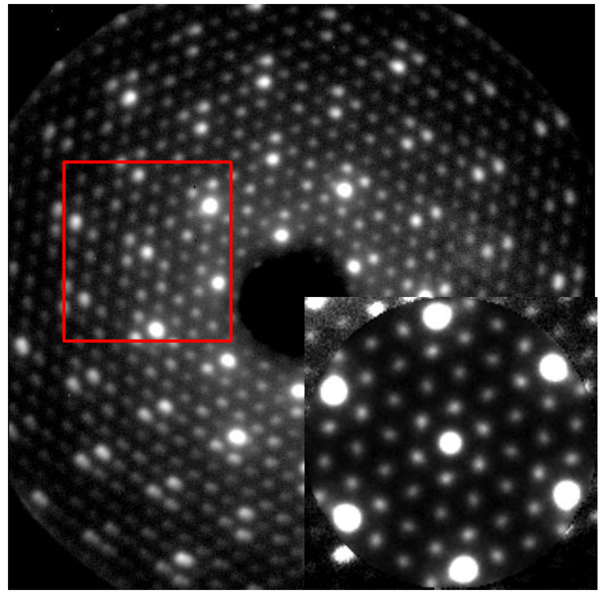


Figure 2: single crystal TaS_2 diffraction.

We also conducted time-resolved experiments on TaS_2. The Bragg's peaks intensity is measured in real time after the sample irradiated by 100fs laser pulses. The preliminary data indicate the occurrence of ~300 fs structural transition, and these results support our estimation of ~100 fs time resolution.

The timing jitter between the pump laser and probe electron beam was experimentally investigated using a RF deflector. Due to the RF break down in the phase, the time resolution of the RF deflector is about 100 fs. By measuring the electron beam centroid position, we concluded that the timing jitter is on the order of 100 fs.

[1] X.J. Wang et al, Proceeding of 2003 Particle Accelerator Conference, 420-422 (2003).

MAJOR MILESTONES:

- FY2012: demonstrate high quality electron diffraction.
- FY2013: 10 Hz operation; performing time-resolved experiments.
- FY2014: improve the time resolution below 100 fs, publish 2 to 4 high impact journal articles. Seeking DOE funding for MeV UED operation.

Femto-Second X-ray Pulse Generation by Electron Beam Slicing

LDRD Project 12-023

Li Hua Yu, T. Shaftan, F. Willeke

PURPOSE:

We propose to investigate femto-second x-ray pulse generation in a storage ring by electron beam slicing. When short electron bunch from linac (5MeV, 50pC, 150fs) passes above a storage ring bunch (30 ps), it kicks a slice (200fs) vertically. The radiation from the short slice is separated from the core bunch [1]. The new method may be used to create ultra-short x-ray pulse in storage rings. There is strong user interest in ultra-short x-ray pulses (see APS upgrade). Our objective is to study the feasibility of this new method. The success of this program will lead to a design of a first test system at NSLS II, with simulation results to compare the new technique with other methods of generation of short x-ray pulses, confirm its advantages, as our initial estimate predicted.

APPROACH:

The new method has many advantages when compared to other schemes. It needs much smaller space in storage ring for the interaction point, compared with crab cavity, as used in APS upgrade. The pulse length (200fs) is much shorter than crab cavity method (1-2ps). The flux per pulse may be increased significantly compared with laser slicing (by a factor of 6-10). The repetition rate can be many orders of magnitude higher than laser slicing (about 10 MHz, compared with 1-10kHz). Compared with LCLS, there is 10^4~10^5 of magnitude higher repetition rate, and the output is much more stable.

As a first step in the development of the new method, in this LDRD proposal**,** we propose to study the first crucial part of this scheme: micro-focusing of low energy electron beam in space charge dominated regime. This simulation study provides a basis as a reference for a more specific design of an electron beam slicing beamline at NSLSII, which will be the second step of our program. The success of this program will have a strong potential to bring the capacity of a storage ring light source to a new high level, and hence is well tied to the DOE mission.

In June of 2012, we hired a post-doc, An He, in the middle of our first step--- the simulation of a chicane structure to compress a very low energy negatively chirped electron bunch in the space charge dominated regime. We also received help from G. Wang, L. Yang, and Y. Hidaka, and other members in our accelerator division. Even though due to the fact that they are committed to the commissioning of NSLS II, and can only spare very small amount of their time to our LDRD program, the discussion and collaboration with them are very valuable and fruitful.

TECHNICAL PROGRESS AND RESULTS:

The first step of the program is to find whether it is possible to obtain electron bunching at 5 MeV with 50 to 100 pC of charge and compress it to 150 fs and 50 micron beam size after a compression chicane. There are mainly two difficulties in this design. The first is that in order to lower the cost of the system, we seek to use only a photo-cathode electron RF gun as the electron beam source without additional RF cavity to accelerate the electron bunch after the RF gun and also without the RF cavity to generate the chirp for the electron bunch. The second is that this is in a space charge dominated domain, so the conventional linear lattice design can only be used as a guideline at the first stage of the study.

By simulation, we confirmed that the energy chirp from RF-gun is small and negative, i.e., the energy of the electron at the head of the bunch has higher energy than the tail. Thus, to compress the bunch, we must use the unconventional magnetic chicane with positive R56 such that the higher energy particles go through a longer path length than the low energy particles so that after the chicane the electrons at the tail with lower energy will be able to catch up the particles at the head of the electron bunch. To reduce the R56, against intuition, instead of avoiding the space charge effect, we focus the electron beam and use this effect to increase the energy chirp to 1%/ps.

Our analysis showed that we have a rather restricted condition for the compressor: we need to control beta function to within 10 m, and require dispersion function to be less than 12 cm, and we need energy chirp near or larger than 1%. We were able to find a configuration of the positive R56 chicane to reach 65mm, which is needed for the compression within a 5 meter distance.

To be able to analyze the performance of the chicane in the charge dominated regime, we developed a concept of equivalent beta function and dispersion, even though these parameters lost their meaning due to space charge, when particle energy is changing as it passes through the system. This concept provided guidance in our optimization process.

During the optimization process, we realized that due to phase space conservation, increased energy spread could lead to reduced bunch length. Thus, again, using space charge effect instead of avoiding it, we further increased the focusing before the entrance to the chicane, and hence further increased energy spread, and finally achieved the compression to 150 fs while the beam size at the focal point reaches 50 micron.

Thus in the first year we have already achieved our goal of the first step: by simulation, we confirmed the feasibility of electron beam slicing using low energy electron bunch. The result is very close to original estimated specification. This provides a solid reference point for the next step, a design of an electron beam slicing beamline at NSLS II.

We plan to carry out the first 4 to 5 steps of the following steps in the next fiscal year:

1. Study whether tilted crossing can reduce the bunch length increase due to horizontal beam size
2. Find an appropriate location in NSLS II ring.
3. Design the beamline and carry out simulation and optimization for the system.
4. RF-gun output energy can be larger than 5MeV, and may be as high as 12 MeV. We will optimize this parameter and we expect the resulting bunch length may be less than 150fs.
5. Find the appropriate beta function at the crossing point.
6. Study the separation from the core in the wiggler radiator
7. Study the radiation opening angle in the soft x-ray range and its relation to separation.
8.

Thermochemical Conversion of Biomass to Fuels and Chemicals

LDRD Project 12-024

Nii Ofei Mante and Suresh P. Babu

PURPOSE:

The purpose of the LDRD project is to identify pathways to evaluate the suitability of commercial and evolving thermochemical conversion (i.e., pyrolysis and gasification) processes to produce efficient and clean forms of renewable fuels, power, chemicals and their co-production where appropriate, employing NY State and NE USA (NYS-NEUS) biomass materials. The initiative will draw upon the existing know-how in fundamental science to techno-economic and sustainability analysis, in Plant Biology, Chemistry, CFN, and Sustainable Energy Technology Divisions. The project should help enhance in house biomass thermochemical conversion R&TD capabilities as well as laboratories that would be necessary to develop patentable efficient and economical process innovations for scale-up investigations.

APPROACH:

In order to commercially produce high-value chemicals and chemical intermediates from biomass, it is known that pyrolyzing (i) low-lignin and high cellulose biomass produces fine chemicals, such as levoglucosan, levoglucosanone, and (ii) high lignin biomass results in high yield of aromatics and miscellaneous monomers and precursors to produce adhesives, binders, resins, and a variety of ligno-sulfonates.

The unresolved technical hurdle in biomass pyrolysis include the wide-range of oxygenates in bio-oil which are unstable and have a low-pH. The LDRD project will extend BNL's nano-structured catalysts for de-oxygenation, conditioning, and stabilization, while the raw pyrolysis products are still in the gaseous state to produce fungible fuels or high-value-chemicals.

Hot- or medium-temperature cleanup of biomass gasification raw product gases is a key unresolved technical hurdle for efficient production of synthesis gas from biomass. The raw gas contaminants include condensable hydrocarbons (tars), particulates, NH_3, alkali, chlorine and sulfur compounds. The LDRD project will extend BNL's proven expertise with CeO_2 and TiO_2 based nano-structured catalysts to simultaneously reform condensable hydrocarbons, CH_4, and NH_3 in order to produce a clean synthesis gas for subsequent conversion to fuels and chemicals. Alkali and chlorine could be removed with biomass ash and sorbents, while particulates are removed employing high-temperature porous membranes.

TECHNICAL PROGRESS AND RESULTS:

RESULTS: The Task 1, base line experiments conducted at ~550^{o} C confirmed that structural building blocks of biomass affected the chemical composition of pyrolysis oil. High yields of levoglucosan and acetaldehyde were produced mainly from pyrolysis of cellulose and from poplar and hot water treated sugar maple. Pure phenol was detected only in the products from willow and switch grass. The lignin pyrolysis products, namely syringyl and guaiacyl derivatives were found to be high with the hardwood samples, poplar producing the highest. However, the significant yields of 2-methoxy-4-vinylphenol and 2,3-dihydrobenzofuran from switchgrass suggest differences between the type of lignin found in herbaceous and woody feedstocks. The lower yields of carboxylic acids produced from the hot water treated sugar maple suggest that the usual high acid number associated with pyrolysis oils can be reduced by engineering plants to produce biomass with lower hemicellulose content.

The primary results from Task 2 on the catalytic stabilization and conditioning of pyrolysis vapors showed that BNL's TiO_2 based nano-structured catalysts promoted ketonization reactions and transformed key decomposition products from cellulose and hemicellulose into cyclopentenone derivatives, acetone and 2-butanone.

PROGRESS: The LDRD project was initiated at the beginning of CY 2012. Research work has begun with the hiring of a Post-Doctoral Researcher in May 2012, Dr. Nii Ofei Mante, who has hands-on research experience with thermochemical conversion of biomass. In the following months the necessary bench-scale research equipment were procured and set-up in Lab D-8, Building 815. In mid-July BNL Experiment Safety Review (ESR) of the CS Analytical 5200 Pyroprobe and Agilent 5975C GC/MS system was completed. This was followed by calibration of the GC-MS analytical equipment. The rest of the experimental research is summarized below.

Task 1. Effect of plant constituents on the primary products of TCC (Task Leader: C.J. Liu)
The following biomass samples, representative of NE biomass that may be available for large-scale commercial conversion to fuels and chemicals, were selected for the LDRD research:

1. Poplar with selected cellulose and lignin contents – To be provided by BNL Plant Biology Department
2. Poplar- (INL)
3. Willow -(INL)
4. Willow -(SUNY ESF)
5. Sugar Maple –with bark- (SUNY ESF)
6. Sugar Maple – without Bark- (SUNY ESF)
7. Hot Water extracted Maple without Bark - (SUNY ESF)
8. Switch-grass (*Panicum virgatum* L.,) - (SUNY ESF)

The base line TGA and ambient pressure flash pyrolysis (with He as carrier gas) experiments were conducted at a peak temperature of 550 C with pure cellulose, Xylan, and lignin in addition to the biomass samples provided by INL and SUNY ESF. The particulars of these experiments along with the TGA and GC-MS profiles of primary products of pyrolysis are available for detailed discussion.

Task 2. Development of catalysts for stabilization/conditioning of primary raw pyrolysis and gasification product streams (Task Leader: W. Han and J. Rodriguez)

BNL CFN provided 2.75 gms of TiO_2 nano-rods as the support for preparing nano-structured catalysts to be developed for stabilization/conditioning of raw biomass pyrolysis and gasification products. The TiO_2 support material was employed by BNL Chemistry material to develop nano-structured catalysts with 1 wt% and 5 wt.% of Ni and Pt. At present these BNL catalyst supports and nano-structured catalysts are being characterized using XRD, XAFS and TEM techniques.

Task 3. Development of catalysts for conversion of CO, CO2, H2, and H2O to mixed alcohols with preference to butanol (Task Leader: J. Rodriguez)

No activity was planned for this reporting period.

Task 4. TEA and the Applicability of Research Results to NYS and NE-US Biomass Utilization:

No activity was planned for this reporting period.

Flow-Based Battery Architectures for Large Scale Electrical Energy Storage

LDRD Project 12-025
Can Erdonmez

PURPOSE:

Flow-assisted battery architectures combine attractive features of fuel cells and battery technology. The applications that these solutions target, particularly in grid-scale energy storage, however, have extremely demanding cost and reliability requirements. The two broad goals of this project are: 1) develop, at BNL, with participation from external collaborators, platforms for advanced materials characterization (both *ex situ* and *in operando*) to shed light on processes that dictate performance and reliability in battery chemistries targeting flow-based energy storage solutions, 2) apply these tools to some promising emerging/re-emerging flow-assisted battery technologies to guide further efforts in both basic and applied research at the interface of electrochemistry and materials science. We believe that the techniques developed and the insights gained will allow us to compete for follow-on funding from EERE, BES & NYSERDA.

APPROACH:

Emerging applications in large-scale electrochemical energy storage require near-order-of-magnitude improvements in cost and lifetime over state-of-the-art technologies, while allowing relaxation of other performance metrics (e.g. energy or power density). Some flow battery technologies, utilizing liquid electrochemical fuels, have become active research areas, but the sacrifices in energy and power density are presently large enough to raise concerns about final systems cost. Additionally, the most developed flow battery chemistries employ active materials that raise questions of long-term resource availability and toxicity. Our belief is that some combination of solid-state active materials and a flow-assisted architecture is more likely to provide the best balance of performance and reliability in the long term.

The investigation therefore focuses on morphological, structural and chemical structure and evolution of solid-state active and supporting materials in flow-based electrochemical systems. Two specific architectures have been chosen as the systems where the bulk of technique development is to take place: 1) flow-assisted alkaline batteries where system architecture focuses on converting a non-rechargeable battery technology into a rechargeable one, 2) Li-ion batteries where the active material takes the form of a slurry-based electrochemical fuel that can be pumped through a reactor, thus decoupling energy density from power performance. These two systems together capture a number of scientific directions and engineering choices emerging from the flow battery field, such as electrodeposited metal anodes, suppression of dendritic microstructures, aqueous *versus* non-aqueous electrolytes, microporous *versus* ion-selective membranes.

We have chosen to pursue the design of electrochemical devices that correspond, as much as possible, to systems intended for eventual industrial production and deployment, while at the same time allowing for study by multiple advanced materials and electrochemical characterization techniques. The co-investigators for this project thus have been chosen to provide expertise on synchrotron characterization (Jun Wang, *NSLS*, *BNL*), advanced electron microscopy (Yimei Zhu, *MSD, BNL*), engineering of slurry-based flow batteries (*Yet-Ming Chiang*, *MIT*) and engineering and characterization of flow-assisted energy storage technologies employing electrodeposition (*Dan Steingart & Sanjoy Banerjee, CCNY*).

TECHNICAL PROGRESS AND RESULTS:

The project start was in June 2012. Thus, this report refers to progress to the initial 4 months of the project in FY12.

Initial tests were completed at NSLS at multiple beamlines (X8C: transmission X-ray microscopy, X13B: microdiffraction, X14A: time-resolved diffraction, X17B: energy dispersive diffraction) utilizing a number of different device form factors of alkaline battery chemistry. For the tests at X8C and X13B, a microfluidic Zn electrodeposition cell was developed to study morphological and phase evolution on Zn anodes. Using these microfluidic cells, *in situ* data from operational electrochemical systems could be collected, a first in the case of these two beamlines. The system design was performed collectively between collaborators at ST (BNL), NSLS (BNL) and CCNY. Thus one of the milestones of the project, the design and construction of flow cells for synchrotron studies of electrodeposition phenomena has been completed. The microfluidic cell and some initial results are included below. The initial results already suggest resolution of some standing questions in Zn deposition in an alkaline environment, regarding e.g. the role of electrolyte dopants in modifying Zn morphology.

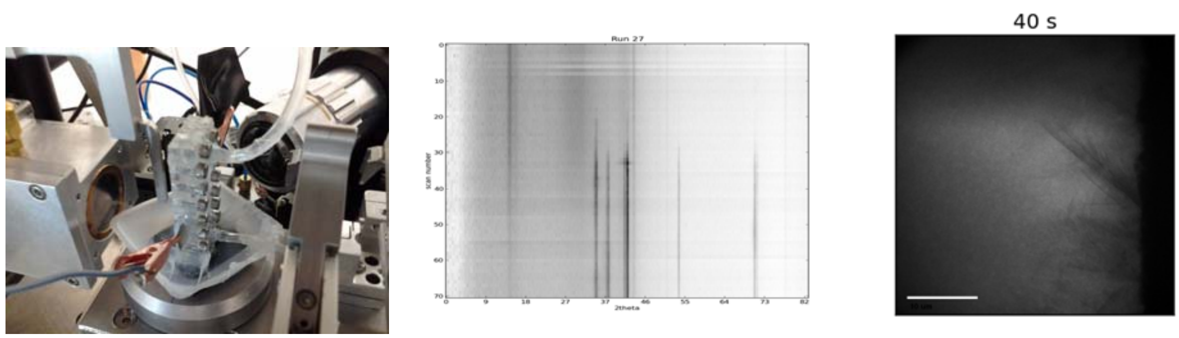


Figure – left: microfluidic electrodeposition cell, middle: time-resolved *in situ* microdiffraction data from electrodeposited metal layer, right: trransmission x-ray microscopy image of electrodeposited non-dense structures, collected in situ from the same cell design.

Milestones for each year of anticipated funding:
FY13 – *in situ* synchrotron studies using microfluidic electrodeposition cells developed; Synchotron studies of cathode material structure and evolution in alkaline environments; preliminary electrochemical studies of alternative flow battery chemistries

FY14 – Initiate synthetic development and characterization of doped and or nanostructured active and supporting materials; use electron microscopy to determine morphology and chemistry of supporting materials in slurry-based electrochemical fuels

FY15 – electron microscopy, synthesis and electrochemical efforts to focus on novel systems (based on either architecture or active material chemistry)

Demonstration of a Grid-Wide Measurement and Control Platform for Micro-Grids

LDRD Project 12-029

M. Villaran, M. Yue, R. Lofaro

PURPOSE:

This project proposes the development and demonstration of an electrical grid measurement and control platform that can be used to monitor and manage electrical distribution systems to improve their reliability and efficiency. The platform will also strive to be capable of establishing and controlling islandable micro-grids from selected portions of a distribution system. The proposed platform will be based on the use of an innovative new smart grid sensor designed specifically for electrical distribution systems that can provide high-speed synchronized measurements of phasor data, power/energy, power quality, harmonics and waveforms from various points in an electrical distribution system and also provide control capabilities [Ref. 1].

The proposed platform will be developed and demonstrated using selected portions of the BNL campus electrical distribution network. As part of the demonstration, a micro-grid capability will be developed at the Northeast Solar Energy Research Center (NSERC) that will include up to 1 MW of renewable generation from its new research solar photovoltaic array. The micro-grid would be representative of such a system, with a significant quantity of renewable energy sources that might be established in large residential developments, industrial complexes, or autonomous DoE or DoD facilities with high energy demand. The experience gained from the performance of this project will help to establish BNL's capabilities in the development of grid measurement and control systems and renewable energy integration technologies.

APPROACH:

The nation's electrical grid is comprised of different elements, including generation sources, transmission systems, distribution systems and finally the end-use loads. In an effort to improve the reliability and efficiency of the grid, there is an ongoing initiative to restructure the existing grid using new smart grid technologies [Ref. 2]. The new Smart Grid will allow a move away from the current centralized power generation model by enabling the integration of distributed generation sources into the grid. It will also allow the implementation of improved control schemes that utilize two-way power flows and demand-response systems. Enabling the development of the smart grid presents many challenges, including development of measurement and control platforms for each element of the grid.

The proposed smart grid measurement and control platform technology will employ the innovative new Smart Grid Sensor (SGS) developed by SEI of Toronto, a collaborator on this project. This demonstration will be the first of three planned phases of increasingly scaled-up applications of the smart grid measurement and control platform that we will be developing, leading up to a third phase in which the technology is demonstrated to be transferable to an existing installed micro-grid system.

In this initial project, four representative distribution circuits have been selected for deployment of the SGSs: the new NSERC facility, one of the NSLS-I feeders (which have experienced power quality problems in the past), the BNL residential area, and one of the new NSLS-II feeders. Eight SGSs will be deployed at the source (Temple Place Substation) and the first major substation down on each of the circuits. The sensors will be integrated with communications network infrastructure along with data collection and visualization software, and tested on the BNL campus to demonstrate and validate their performance.

In addition to SEI and their smart grid sensor fabricator, Hitachi High Tech of Japan, other collaborators include Electrical Distribution Design (EDD) of Blacksburg, Virginia, and Orange and Rockland Utilities (ORU) of Spring Valley, New York.

TECHNICAL PROGRESS AND RESULTS:
The program plan was developed [Ref. 3] and BNL is working toward developing the connection details for deploying smart grid sensor (SGS) instruments on the four demonstration distribution feeders. The design for residential area feeder is complete, the hardware has been built, and is awaiting final installation (see photos of instrument enclosure for Substation 616). Fiber optic communication link upgrade to the residential substation 616 has been completed. Designs for the other three demonstration feeders are under way.

Photographs: P. Giannotti

SGS Enclosure for Substation 616: front view, left; internal wiring, right.

Eight (8) test-only smart grid sensors have been received from SEI, Inc. and BNL and Orange & Rockland Utilities are developing preinstallation tests. Manufacture of the first functional field-ready SGS instruments is delayed, but should not affect instrument field connection design and installation significantly. SEI is finalizing SGS instrument firmware.

Simulation modeling, using DEW/ISM software, of the demo feeders is underway; work is being coordinated with interfacing project efforts for SGRID3 and AEGIS Center initiatives at BNL.

REFERENCES:

1. Smart Energy Instruments, SEI Smart Grid Sensor Technology Brief, 2011
2. US Department of Energy- Office of Electricity Delivery & Energy Reliability, Smart Grid Research & Development Multi-Year Program Plan 2010-2014, 2nd Draft, March 2010.
3. Program Plan: Development and Demonstration of a Smart Distribution Grid Measurement and Control Platform, Rev 0. Brookhaven National Laboratory, April 26, 2012.

Laser-Driven Proton Accelerator

LDRD Project 12-032

Igor Pogorelsky

PURPOSE:

The main goal of the project is to optimize proton beams generated by the interaction of a high power laser pulse focussed in a hydrogen gas jet. The maximum proton energy is expected to increase from 2 MeV to ~10 MeV with proportional increase in the CO_2 laser driver intensity. These developments will serve as steps to the next-generation of ultra-fast mid-IR lasers; provide insights into the fundamentals of laser/plasma interactions; and verify energy scaling laws for laser driven proton acceleration. The research will also provide necessary arguments to obtain funding for the BNL/SUNYSB initiative aimed at developing a compact and economical alternative source for hadron cancer therapy.

APPROACH:

By a string of innovations, we plan to increase the CO_2 laser intensity by one order of magnitude. This include: femtosecond optical parametric generator based on a Ti-Sapphire laser and Chirped Pulse Amplification (CPA) technique that has never been attempted with molecular gas lasers. Concurrent to the laser improvements, we will engage into the optimization of the proton beam generation process. We will introduce a novel method of enhancing the acceleration process by using two laser pulses with a variable time delay.

The team of investigators assembled to conduct this project includes: the PI, M. Polyanskiy, M. Babzien, O. Tresca from the ATF and users from SUNYSB C. Mahrajan and N. Cook.

TECHNICAL PROGRESS AND RESULTS:

We report on technical progress according to the three milestones identified in the LDRD proposal:

<u>Milestone 1</u> “Process simulation specific for the ATF experimental conditions”.

- By PIC simulations, illustrated in Fig.1, we confirmed our initial suggestion regarding the need for proper plasma target preparation – that is steepening of the leading front in the gas-jet plasma density distribution before arrival of the accelerating laser pulse. Such steepening will be accomplished by a snow-plow effect caused by an auxiliary CO_2 laser pulse, preceding the main accelerating pulse and properly tailored in energy and time delay.
- Following the simulations findings, a pulse splitter has been built into the laser chain and generation of two amplified laser pulses with a variable time delay has been verified.
- Simultaneously, we improved our optical probe diagnostic system that now visualizes the plasma in two moments, when the auxiliary and accelerating CO_2 laser pulses arrive.

<u>Milestone 2</u> “Shortening of the CO_2 laser pulse by using optical parametric amplifier (OPA)”.

- OPA has been installed and characterized for the output parameters and stability. Parameters of this device, 400 □J, 400 fs, and 2 ps timing jitter, are far superior to the previous 10-□m seed pulse injector. This unit has a high repetition rate, and is compact and user-friendly. This is important for prototyping a future laser system for cancer therapy.
- We started tests on the injection and amplification of the OPA pulse through our amplifier chain. This task is in its early stage and is scheduled for reporting later on.
- The currently available diagnostic, a streak camera, is limited in resolution to 6 ps. We now expect much shorter pulses, close to 1 ps, after amplification of a femtosecond seed. We are in a process of building an autocorrelator to measure such ultra-short pulses.

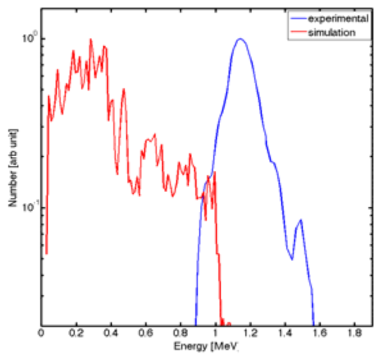


Figure 1. Proton beam spectra show the advantage of a steep plasma density gradient in experiment over ramped plasma density in simulations.

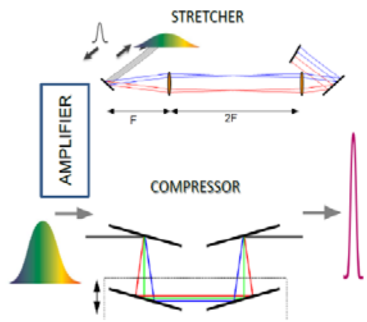


Figure 2. Diagram of a stretcher and compressor built to facilitate laser amplification using the CPA technique.

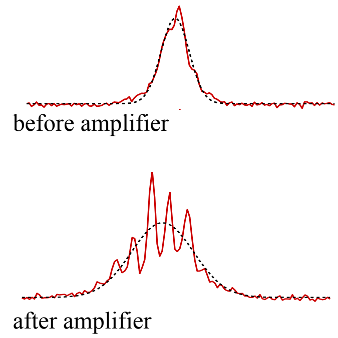


Figure 3. Demonstrated spectrum broadening after amplification; Fourier transformation implies a pulse shortening from 6 ps to 3 ps.

Milestone 3 "Building and testing laser pulse stretcher and compressor".

- The initial low-power stretcher/compressor setup is assembled (see Fig.2). Test of the CPA technique with a CO_2 laser pulse will be carried out in the near future. If the design is successful, we will build a final compressor for the total amplified laser energy that requires bigger diffraction gratings placed under vacuum.

Additional accomplishments

- Via simulations and tests, we improved the performance of our final amplifier. Pulse shortening from 6 to 3 ps during amplification in the saturation regime is confirmed indirectly by spectral measurements (see Fig.3).
- Proton acceleration chamber setup has been improved. A new high-sensitivity proton diagnostic is installed.
- With the doubled laser intensity, laser beam reflections from the plasma were observed. These reflections are amplified as they pass through the amplifiers resulting in damage to critical optical components. This problem was corrected by installing a Ge switch after the amplifiers to block the reflected beam. The switch is controlled by a Nd:glass laser specially procured for this purpose. (See Fig.4 for physical principle of the switch operation.)

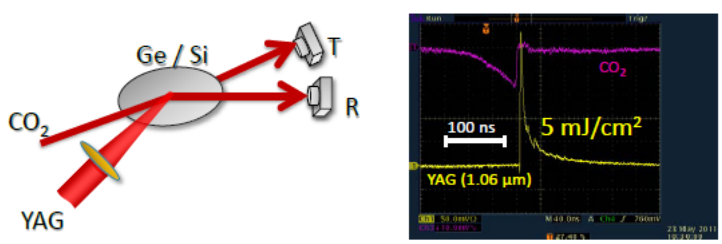


Figure 4. Normally high transmission of CO_2 laser beam through a semiconductor wafer placed at the Brewster angle is stopped abruptly (purple trace) when irradiated by a YAG laser pulse. We use this effect to block parasitic reflections of CO_2 laser beam from plasma.

Action items for next FY.

- Experimental confirmation of the proportional scaling of the accelerated protons energy with increased CO_2 laser beam intensity. Demonstration of >10 MeV monoenergetic proton beams.
- Development of a collaboration for experiments with biological and live tissues.
- Simulations of the regime for generation of monoenergetic proton and ion beams tunable to ≥200 MeV.
- Preparing a proposal for a laser-hadron cancer therapy research facility.

Water-Based Liquid Scintillator Detector for Neutrino and Proton Decay Experiments

LDRD Project 12-033

David Jaffe

PURPOSE:

We are evaluating water-based liquid scintillator (WbLS) as a detection medium using prototype detectors and simulation. New techniques developed by the BNL nuclear chemistry group for making WbLS allow the fraction of scintillating liquid in water to be varied. The primary goal is to measure the light yield for different WbLS formulations with various types of particles with a range of incident energy. The results will allow an assessment of WbLS for potential particle physics experiments such as the search for proton decay ($p \rightarrow K^{+}\nu$) in a large volume detector, low energy neutrino detection using inverse beta decay and dosimetry monitoring.

APPROACH:

Liquid scintillator (LS)-based detectors have demonstrated success in the detection of rare processes. For example large LS-based detectors enabled the discovery of the neutrino, the measurement of the solar neutrino flux and the observation of neutrino interactions. Compared to LS, WbLS benefits from better material compatibility, lower cost, longer attenuation length and fewer hazards related to storage of large quantities of chemicals in underground laboratories.

We have developed two prototype detectors and a data-acquisition system to understand the response of different formulations of WbLS to a low energy proton beam at the NASA Space Radiation Laboratory (NSRL) at BNL, cosmic ray muons and radioactive sources. The scintillation light depends on the particle type and its ionization density. In addition, particles that travel faster than the light in a medium produce light by the Cerenkov process. The relative rates of light production of these processes can be assessed by adjusting the energy of the proton beam. Cosmic rays and radioactive sources will allow use to compare the light yield of different WbLS formulations.

In addition to the PI, collaborators on this work are D. Beznosko, a postdoc hired with LDRD funds, M.Diwan, H.Themann, E.Worcester, B.Viren, and C.Zhang of the BNL Physics Department and S.Hans, R.Rosero and M.Yeh of the BNL Chemistry Department.

TECHNICAL PROGRESS AND RESULTS:

In FY2012, postdoc D.Beznosko was hired and materials and electronics were purchased for the prototype detectors. The detectors were assembled and commissioned with the data acquisition system (DAQ) first in the Physics Department and then at NSRL. Five hours of proton beam data were acquired at NSRL in October. Software for analysis and simulation of the proton beam data was developed. The detectors and DAQ were returned to the physics department and reconfigured for data-taking with cosmic rays and radioactive sources. Preliminary proton beam results are shown in Figure 1 for one of the prototype detectors.

Only the highest proton beam energy produces Cerenkov light in water. The lower light yield for the lower energies in water in Fig. 1 is hypothesized to be due to “knock-on electrons”.

Simulation is being developed to investigate this hypothesis. It is well-known that scintillation light yield is suppressed by higher ionization density. The lower energy protons lose energy by ionization more rapidly. The preliminary results confirm the suppression, but the apparent dependence of the suppression on the LS concentration, as indicated by the convergence of the red and blue curves, is unexpected. Further data analysis and simulation are in progress to improve the understanding of the proton beam results.

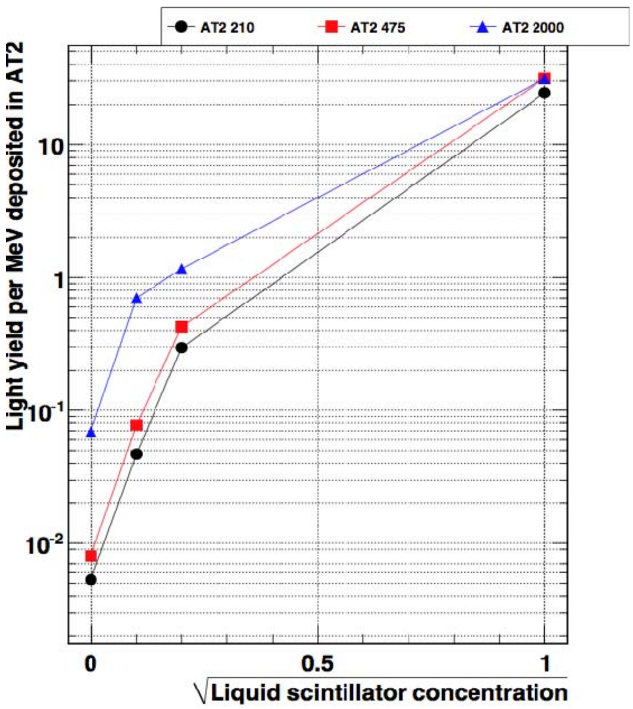


Figure 1: The measured average light yield in arbitrary units divided by the energy deposited as a function of the square root of LS concentration for one of the prototype detectors. The black circles, red squares and blue triangles represent the data acquired with proton beam kinetic energies of 210, 475 and 2000 MeV, respectively. The energy deposit is calculated based on the expected energy loss in the materials in the proton beam. Concentrations of 0 and 1 correspond to pure water and LS, respectively.

We intend to complete and publish the analysis of the 2012 NSRL data in the next few months. With the cosmic ray and radioactive source data, we will measure the light yield for a larger number of WbLS concentrations. A second run at NSRL in Spring 2013 has been proposed and tentatively approved. These data, along with simulation, should allow us to assess the feasibility of large volume WbLS detectors.

Quantum Electrodynamics for QCD Precision Studies at an EIC

LDRD Project 12-034

Marco Stratmann (PI), Elke Aschenauer, Hubert Spiesberger

PURPOSE:

The main purpose of the LDRD project is to develop and provide a comprehensive and reliable set of computational tools to control additional photon radiation to a level of precision necessary to meet the objectives of the physics program laid out for a future electron-ion collider (EIC) such as the eRHIC project at BNL. Quantum Electrodynamics (QED) radiative corrections are known to often reach a level of 100%, affect all measurements with electromagnetic probes, and greatly complicate the experimental reconstruction of relevant kinematic variables and the extraction of vital new information on the structure of hadrons. The anticipated results of this LDRD project will help to understand in detail limitations due to QED radiative effects on key measurements at an EIC and will have impact on certain detector performance requirements.

APPROACH:

The key element of devising strategies to systematically unfold QED radiative corrections from the physics observables of interest is the availability of flexible Monte-Carlo simulations of additional photon radiation in electromagnetic processes that can be easily merged with programs simulating the detector acceptance and response. While the project can benefit from the expertise acquired during DESY-HERA operations, existing programs, and results in the literature, these can serve only as a starting point. A number of potentially important effects and contributions for the EIC physics program, such a polarization effects, are either not available or not in a form which can be implemented into required Monte-Carlo event generators. The main part of this LDRD project is devoted to fill in these gaps by providing missing analytical calculations and developing comprehensive software implementations of QED radiative corrections, tailored to the needs of a future EIC physics program.

Among the most important issues, which require detailed studies, we have identified QED radiative corrections for lepton-nucleon scattering with polarized beams and lepton-nucleus scattering (both have never been studied in a high-energy collider environment) and the role of two-photon processes in measurements of deeply-virtual Compton scattering (DVCS). DVCS is one of the key processes at an EIC to obtain a three-dimensional image of the nucleon structure. To provide missing analytical calculations and turning them into Monte Carlo event generators are the milestones for our LDRD project. Based on the numerical codes, we will study whether kinematic variables can be reconstructed in such a way that QED radiative corrections can be unfolded with the required precision to achieve the goals of a future EIC in spin physics, three-dimensional imaging of the nucleon, and the physics of gluon saturation.

The project benefits greatly from having H. Spiesberger from Mainz, Germany, as one of its investigators. He is one of the few leading experts on simulations of QED radiative corrections and has developed several of the existing codes used at DESY-HERA. The EIC task force at BNL led by E. Aschenauer provides the necessary matching with detector simulations. All studies are done in close collaboration with the BNL EIC task force. In particular, the ability to detect the hadronic final state may prove critical to reduce QED radiative effects at an EIC.

TECHNICAL PROGRESS AND RESULTS:
The project is in its first year of funding and a postdoctoral researcher was hired in June 2012 to work mainly on two-photon processes relevant for future precision measurements of DVCS.

In FY12, we have completed the development of a new event generator for polarized lepton-nucleon scattering by extending the capabilities of existing software for corresponding unpolarized processes. The numerical implementation is in its final validation stage and can be readily linked with detector simulation tools. The availability of the code is a first milestone of our project.

We have also finished work on projections of the impact of future EIC measurements on our knowledge of the spin structure of the nucleon (paper published in Physical Review D and in workshop proceedings; in collaboration with Rodolfo Sassot, Buenos Aires).

In FY12, we have also started to compute two-photon processes in the context of DVCS, and first intermediate results are available. These results are currently being implemented in a first version of a novel event generator to learn about potential numerical issues or subtleties.

In FY13, we fully exploit the developed event generator for polarized lepton-nucleon scattering in several detailed numerical studies of QED radiative corrections to determine how well the unfolding procedure works for various processes. A particular emphasis is on high momentum transfer, charged-current electroweak processes, which require a full reconstruction of the hadronic final state to determine the relevant kinematic variables. The completion of these studies is another milestone of the project.

We continue our work towards analytical expressions for two-photon processes and their implementation into a novel event generator.

We look into QED radiative corrections for lepton-nucleus scattering and their implementation into event generators.

In FY14 (funding for a postdoctoral researcher available until May 2014), we plan to complete our studies of two-photon processes and their impact on measurements of DVCS. This is the final milestone of the project.