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Brookhaven National Laboratory's

Annual Report of

Laboratory Directed Research & Development Program Activities For FY 2000

Director's Office

BROOKHAVEN NATIONAL LABORATORY
BROOKHAVEN SCIENCE ASSOCIATES
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DISCLAIMER

Acknowledgments

The Laboratory Directed Research and Development (LDRD) Program is managed by Leonard Newman, who serves as the Scientific Director, and by Kevin Fox, Special Assistant to the Assistant Laboratory Director for Finance & Administration (ALDFA). Preparation of the FY 2000 report was coordinated and edited by Leonard Newman and Kevin Fox, who wish to thank D.J. Greco and Regina Paquette for their assistance in organizing, typing, and proofing the document. A special thank you is also extended to the Photography and Graphic Arts 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

Brookhaven National (BNL) Laboratory is a multidisciplinary laboratory that carries out basic and applied research in the physical, biomedical and environmental sciences, and in selected energy technologies. It is managed by Brookhaven Science Associates, LLC, under contract with the U. S. Department of Energy. BNL's total annual budget has averaged about $407 million, and its facilities are book valued at over $3.8 billion. There are about 3,000 employees, and another 4,500 guest scientists and students who come each year to use the Laboratory's facilities and work with the staff.

The BNL Laboratory Directed Research and Development (LDRD) Program reports its status to the U.S. Department of Energy (DOE) annually in March, as required by DOE Order 413.2, "Laboratory Directed Research and Development," March 5, 1997, and the LDRD Annual Report guidance, updated February 12, 1999. The LDRD Program obtains its funds through the Laboratory overhead pool and operates under the authority of DOE Order 413.2.

The goals and objectives of BNL's LDRD Program can be inferred from the Program's stated purposes. These are to (1) encourage and support the development of new ideas and technology, (2) promote the early exploration and exploitation of creative and innovative concepts, and (3) develop new "fundable" R&D projects and programs. The emphasis is clearly articulated by BNL to be on supporting exploratory research "which could lead to new programs, projects, and directions" for the Laboratory.

As one of the premier scientific laboratories of the DOE, BNL must continuously foster groundbreaking scientific research. At Brookhaven National Laboratory one such method is through its Laboratory Directed Research and Development Program. This discretionary research and development tool is critical in maintaining the scientific excellence and long-term vitality of the Laboratory. Additionally, it is a means to stimulate the scientific community, fostering new science and technology ideas, which is a major factor in achieving and maintaining staff excellence and a means to address national needs within the overall mission of the DOE and BNL.

The LDRD Annual Report contains summaries of all research activities funded during Fiscal Year 2000. The Project Summaries with their accomplishments described in this report reflect the above. Aside from leading to new fundable or promising programs and producing especially noteworthy research, they have resulted in numerous publications in various professional and scientific journals and presentations at meetings and forums.

All FY 2000 projects are listed and tabulated in the Project Funding Table. Also included in this Annual Report in Appendix A is a summary of the proposed projects for FY 2001. The BNL LDRD budget authority by DOE in FY 2000 was $6 million. The actual allocation totaled $5.5 million.

The following sections in this report contain the management processes, peer review, and portfolio's relatedness to BNL's mission, initiatives, and strategic plans. Also included is a metric of success indicators.

Management Process

PROGRAM ADMINISTRATION:

Overall Coordination: Overall responsibility for coordination, oversight, and administration of BNL's LDRD Program resides with the Laboratory's Director. Day-to-day responsibilities regarding funding, oversight, proposal evaluation, and report preparation have been delegated to the dedicated Scientific Director for the LDRD Program. This is a new position which was deemed necessary to handle the growing LDRD Program and all of its requirements. The Office of the Assistant Laboratory Director for Finance & Administration continues to assist in the administration of the program. This includes administering the program budget, establishment of project accounts, maintaining summary reports, and providing reports of Program activities to the DOE through the Brookhaven Area Manager.

Responsibility for the allocation of resources and the review and selection of proposals lies with a management-level group called the Laboratory Directed Research & Development Program Committee. For Fiscal Year 2000, the Program Committee--which selected the 2001 programs--consisted of eight members. The Laboratory's Deputy Director for Science & Technology chaired the Committee. The other members were five Associate Directors of the Laboratory and two members from the scientific departments and divisions.

2000 LDRD PROGRAM COMMITTEE

Peter Paul	**Chairperson**
Teresa Fryberger	**Energy, Environment & National Security**
Thomas Kirk	**High Energy & Nuclear Physics**
Nora Volkow	**Life Sciences**
Richard Osgood	**Basic Energy Sciences**
Satoshi Ozaki	**RHIC**
Hans Ludwig	**Energy Science**
David Siddons	**National Synchrotron Light Source**

Allocating Funds: There are two types of decisions to be made each year concerning the allocation of funds for the LDRD Program. These are: (1) the amount of money that should be budgeted overall for the Program; and (2) of this, how much, if any, should go to each competing project or proposal. Both of these decisions are made by high-level management.

For each upcoming fiscal year the Laboratory Director, in consultation with the Assistant Laboratory Director for Finance & Administration, develops an overall level of funding for the LDRD Program. The budgeted amount is incorporated into the Laboratory's LDRD Plan, which formally requests authorization from the DOE to expend funds for the LDRD Program up to this ceiling amount.

The majority of projects are authorized for funding at the start of the fiscal year. However, projects can be authorized throughout the fiscal year, as long as funds are available and the approved ceiling for the LDRD Program is not exceeded.

The actual level, which may be less, is determined during the course of the year and is affected by several considerations including: the specific merits of the various project proposals, as determined by Laboratory management and the members of the LDRD Program Committee; the overall financial health of the Laboratory; and a number of budgetary tradeoffs between LDRD and other overhead expenses. At BNL the LDRD Program (see table below) has historically amounted to a much smaller portion of the total budget than at comparable national laboratories. This prevented the Laboratory from preparing itself for work in emerging areas of research. Accordingly, this fraction of LDRD funds is being increased with a target of about 4%.

LDRD COSTS VS. TOTAL LABORATORY COSTS

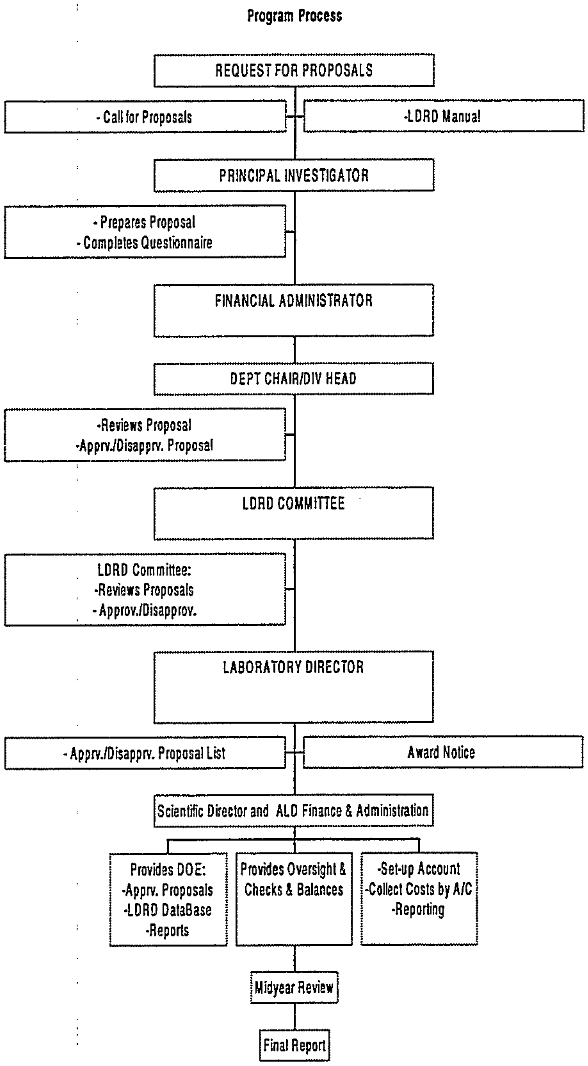
operating $ in millions

FISCAL YEAR	DOE FUNDS	WFO FUNDS	TOTAL FUNDS	LDRD FUNDS	% OF TOTAL
1985	153.0	40.4	193.1	1.82	0.9
1986	156.5	45.1	201.6	2.52	1.2
1987	161.7	45.6	207.3	1.44	0.7
1988	176.7	45.9	222.6	1.51	0.7
1989	193.6	46.7	240.3	2.67	1.1
1990	203.8	45.2	249.0	1.94	0.8
1991	220.9	50.3	271.2	1.32	0.5
1992	234.3	47.2	281.5	1.87	0.7
1993	231.4	47.3	278.7	2.01	0.7
1994	237.0	47.9	284.9	2.32	0.8
1995	243.0	53.7	296.7	2.48	0.8
1996	251.6	50.6	302.2	3.05	1.0
1997	257.2	52.5	309.7	3.46	1.1
1998	251.8	49.5	301.3	2.56	.8
1999	294.1	48.1	342.2	4.53	1.3
2000	343.0	58.0	401.0	5.58	1.4
2001	356.0	99.0	455.0*	6.00	1.3

*Estimated only

Request for Proposals: The availability of special funds for research under the LDRD Program is well publicized throughout the Laboratory. This is done using two methods --one occurring at yearly intervals, the other occurring irregularly. Each year a call memorandum is sent by the Laboratory Deputy Director to all the Associate Laboratory Directors and Department Chairpersons. The FY 2000 call memorandum is attached as Exhibit A. For FY 2001 this call memorandum was issued in January 2000. This early schedule better facilitated the recruitment of post-doctorate candidates to support LDRD projects. Both memorandums reference the BNL LDRD Manual, which is available to all employees on the web at https://sbms.bnl.gov/ld/ld03/ld03d011.htm. (Exhibit B) The other method is by announcement in The Bulletin, the Laboratory's weekly newspaper.

The LDRD Manual specifies the requirements necessary for participation in the program. It states the program's purpose, general characteristics, procedures for applying, and restrictions. An application for funding, i.e., a project proposal, takes the form of a completed "Proposal Information Questionnaire," Exhibit C. An application must be approved up the chain-of-command which includes the initiator's Department or Division Budget Administrator and the Department Chairperson or Division Head. Plans to ensure the satisfactory continuation of the principal investigator's regularly funded programs must also be approved. The applications are then forwarded to the LDRD Program Committee for full review and consideration for funding.



The process that solicits and encourages the development of proposals has evolved into two modes of operation. Specifically, the ideas for proposal development may originate among the scientific staff in response to the general call for proposals. Alternatively, they may be initiated by Laboratory science management. Eventually, both follow the standard procedures for proposal approval up the chain-of-command to the same decision makers. The fact that all proposals must be approved up the chain-of-command permits BNL managers to consider all ideas together when designing the mix of projects for the LDRD Program.

An initiative from management typically takes the form of a broad topical area or item of special interest such as nanoscale science. Then ideas are communicated to a group of scientific staff, who is known to be in a position to pursue and develop the idea in the form of a more formal proposal.

Proposal Review: Once the cognizant line managers approve the proposals, they are forwarded to the Chairperson of the Committee who transmits a copy of all proposals received to the Committee for review. The Committee considers all proposals that have met certain minimum requirements pertaining to the Department's and BNL's LDRD policies.

Lead proponent responsibility of a proposal is assigned to that Associate Laboratory Director of the Committee who oversees and directs the technical area from which the proposal originated. All members have several weeks to review the proposals and prepare for the full debate of the proposal.

Selection Criteria: Minimum requirements of each proposal are: (1) consistency with program purpose; (2) consistency with missions of BNL, DOE, and NRC; (3) approval by Department Chairperson and/or Division Head, and cognizant Associate/ Assistant Director; (4) assurance of satisfactory continuation of principal investigator's regularly funded programs; (5) modest size and limited to 3 years; (6) will not substitute for, supplement, or extend funding for tasks normally funded by DOE, NRC, or other users of the Laboratory; (7) will not require the acquisition of permanent staff; (8) will not create a commitment of future multi-year funding to reach a useful stage of completion; and (9) will not fund construction line-item projects, facility maintenance, or general purpose capital equipment.

The selection criteria used to evaluate and rank individual proposals are stated in broad terms. While the LDRD Manual clearly states that selection is based on (1) scientific or technological merit, (2) innovativeness, (3) compliance with minimum requirements, (4) proposal cost as compared to the amount of available funding, and (5) its potential for follow-on funding. The requirements of DOE Order 413.2 are also carefully considered during the selection process to ensure that proposals are consistent with DOE criteria.

Project Approval: After all presentations are heard, the Committee selects the highest priority proposals by concurrence. Differences, if any, are resolved by the Chairperson. Some funding may be held in reserve during the earlier meetings of the fiscal year so that funds remain available for proposals submitted at later dates. The funding amount requested in any one specific proposal may be changed or adjusted during the approval process. The Committee's recommendation is then submitted to the Director for his approval. The Assistant Laboratory Director for Finance & Administration then sets up a separate Laboratory overhead account to budget and collect the costs for the project.

Project Supervision: The Scientific Director for LDRD carries out overall supervision of the projects. Supervision over the actual performance of LDRD projects is carried out in the same way as other research projects at the Laboratory. Each principal investigator is assigned to an organizational unit (Department, Division), that is supervised by a chairperson or manager.

Each chairperson or manager is responsible for seeing that the obligations of the principal investigator are satisfactorily fulfilled and that the research itself is carried out according to standard expectations of professionalism and scientific method. The Scientific Director monitors the project's status, schedule, and progress and coordinates with the chairperson or manager as necessary.

The Scientific Director of LDRD and Chairperson of the LDRD Program Committee perform a mid-year review of all projects. This review checks on the progress of the projects including its funding schedule. The Scientific Director of LDRD ensures that the work is completed in a timely manner and that annual status reports are submitted to the Director.

In addition, The Scientific Director conducts a monthly meeting with the DOE Brookhaven Area Office to update the progress of the program and to solicit assistance to verify that the BNL LDRD Program is meeting the overall LDRD requirements. This includes providing the DOE Brookhaven Area Office with copies of all funded proposals, an LDRD Program database, and a project funding and schedules summary report.

Project Reporting: Routine documentation of each project funded under the LDRD Program consists of a file containing: (1) a copy of the written proposal; (2) all interim status reports; (3) notifications of changes in research direction, if any; and (4) reports on costs incurred. Also, a formal Annual Report on the LDRD Program is submitted to BNL management and the DOE, summarizing work progress, accomplishments, and project status on all projects.

Documentation for the overall Program consists of (1) various program history files, (2) a running list of all proposals with their acceptance/rejection status, (3) funding schedule and summary reports for all approved projects, (4) permanent records on cost accounting, and a database containing information on each funded project (description, funding by fiscal year, status and accomplishments, follow-on funding, publications, etc.).

Some of the projects involve animals or humans. Those projects have received approval from the Laboratory's appropriate review committees. The projects which involve animals or humans are identified in this report as follows:

Note: This project involves animal vertebrates or human subjects.

This is noted on the summary sheet and also at the end of each report.

Peer Review

LDRD projects have peer reviews performed in several different ways. Primary LDRD research is managed and reviewed by the Laboratory's Department and Division management. These projects are a part of the activities of their respective Department and Divisions in which they reside. The BNL LDRD Program itself does not solicit formal peer reviews, consisting of written comments by experts outside the normal lines of supervision. Instead, advisory committees that consist of subject matter experts from academia and industry conduct peer reviews of LDRD projects as part of a department 's program review. One such group is the Brookhaven Science Associates' Science Advisory Committee, which performs peer reviews of different Laboratory programs on a rotating basis.

In addition to these outside peer reviews of the BNL program, the members of the LDRD Committee are considered to have sufficient technical knowledge to perform peer reviews of projects during the initial selection process and annual renewal. Also, all LDRD projects go through a formal mid-year review conducted by the Scientific Director of the LDRD Program and includes the appropriate Department Chair and Associate Laboratory Director.

Results: The BNL LDRD Program clearly has a vested interest in performing peer reviews in order to maintain a high caliber of research. The results of these reviews are included in the BNL Year End Self-Evaluation for Fiscal Year 2000.

Brookhaven Science Associates (BSA) operates BNL utilizing a Performance-Based Management System (PBMS). The PBMS is designed to include a hierarchy of clear, reasonable, and objective performance measures as standards to assess BSA's overall performance of scientific, technical, operational, community, and managerial (and communications) obligations.

Specifically, in FY 2000 BNL had four critical outcomes in the BSA Contract. The most important critical outcome was Excellence in Science and Technology. Under this critical outcome was an objective entitled Quality of Research. LDRD projects were included in the self-evaluation for this objective.

In the evaluation process the Associate Laboratory Directors (ALDs) of the four BNL Science Directorates assigned self-evaluation scores for each of the four Critical Outcome Objectives, which are Quality of Research, Relevance to DOE Mission and National Need, Success in Construction and Operation of Research Facilities, and Effectiveness and Efficiency of Research Program Management. In determining the evaluation scores the ALDs considered many factors, including bench-marks from past experience and DOE evaluations, major successes such as the RHIC startup and hiring of scientific staff, peer review input, and on the negative side research program deficiencies, such as the conditions that warranted the human subjects research program stand-down.

For FY 2000, the performance under this Critical Outcome was an Outstanding with an overall score of 3.65 out of a possible 4.0.

Relatedness of LDRD to Laboratory Programs and Initiatives

BNL's mission is to produce excellent science in a safe, environmentally benign manner with the cooperation, support, and appropriate involvement of our many communities. Brookhaven was founded as a laboratory which would provide specialized research facilities that could not be designed, built and operated at a university or industrial complex, and provides a scientific core effort for these facilities. This still remains a basic mission of the Laboratory.

BNL is committed to cultivating programs (including the LDRD) of the highest quality. These programs address DOE's Strategic Mission which is to conduct programs relating to energy resources, national nuclear security, environmental quality, and science.

Brookhaven National Laboratory has the following four elements to its mission which support the four DOE programmatic business lines.

RESEARCH FACILITIES
Conceive, design, construct, and operate complex, leading-edge, user-oriented facilities in a safe and environmentally benign manner that is responsive to the DOE, and the needs of the users.
SCIENTIFIC RESEARCH
Carry out basic and applied research in long-term programs at the frontier of science that supports DOE missions and the needs of the Laboratory's users community.
TECHNOLOGY DEVELOPMENT
Develop advanced technologies that address national needs and initiate their transfer to other organizations and to the commercial sector.
KNOWLEDGE TRANSFER
Disseminate technical knowledge to educate new generations of scientists and engineers, to maintain technical currency in the nation's workforce, and to encourage scientific awareness in the general public.

Research Facilities and Scientific Research have a synergistic relationship. To maintain and constantly improve a research facility, and to keep it at the cutting edge, it is essential that the Laboratory have a significant research staff of excellent stature. The staff drives the performance of the facility. Having several complementary facilities at one location, such as the National Synchrotron Light Source and the Alternating Gradient Synchrotron, allows unique research capabilities. The other two elements of the Laboratory's mission--Technology Development and Knowledge Transfer-- bridge all of the research facilities and research programs.

The four elements of Brookhaven's mission support and cut across the four central activities of the Department of Energy as defined in its Strategic Plan.

The Laboratory's breadth of expertise as delineated in Table 1 and 2 provides the basis for its contributions to the DOE's missions and focuses on providing extraordinary tools for the pursuit of basic science and technology.

Table 1 - Expertise Derived from Brookhaven's Core Competencies - Science

High Energy and Nuclear Physics:
- Rare kaon decays
- Muon anomalous magnetic moment
- Exotics and glueball spectroscopy
- Strange matter
- Solar neutrinos
- Nuclear matter in extremes of temperature and density
- QCD phase transitions

Advanced Accelerator Concepts:
- Short wavelength accelerating structures
- Production of coherent radiation free electron laser
- Muon collider and storage ring
- Neutron Sources
- Interlaboratory collaboration on the design and construction of the Spallation Neutron Source

Materials Sciences:
- High Tc superconductivity
- Magnetism
- Surface studies-catalysis, corrosion and adhesion
- Condensed matter theory: metallic alloys and correlated electron systems
- Materials synthesis and characterization with neutron- and X-ray diffraction
- Structure and dynamics
- Defect structure

Chemical Sciences:
- Dynamics, energetics, reaction kinetics on the pico-second time scale
- Thermal-, photo- and radiation-reactions
- Catalysis and interfacial chemistry
- Homogeneous catalysis with metal hydrides
- Porphryin chemistry
- Electrochemistry

Environmental Sciences:
- Global change
- Atmospheric chemistry
- Marine science
- Soil chemistry
- Cycling of pollutants
- Environmental remediation

Medical Science:
- Medical imaging: PET, MRI, SPECT, Coronary Angiography
- Nuclear medicine
- Radionuclides, radiopharmaceuticals, synthesis and application
- Advanced cancer therapies: neutron capture, microbeam radiation, proton radiation, photon-activation therapy
- Mechanisms of oncogenesis

Molecular Biology and Biotechnology:
- Genome structure, gene expression, molecular genetics
- DNA replication, damage and repair
- Structure and function of enzymes, protein engineering
- Plant genomics, biochemistry and energetics
- Solution structure, kinetics and interaction of biomolecules
- Biostructure determination by X-ray and Neutron scattering
- Biostructure determination and mass measurements by electron microscopy

Advanced Scientific Computing and Systems Analysis:
- Atmospheric Transport Modeling
- Infrastructure assessment
- Energy modeling
- Groundwater modeling
- Intelligent sensor and security systems

Table 2 - Expertise Derived from Brookhaven's Core Competencies - Technology

Physical, Chemical and Materials Science:
- Advanced instrumentation and devices for precision electronics, optics and microelectronics
- Superconducting and magnetic materials
- Micromachining
- Battery technology
- Permanent magnets
- "Designer" polymers

Accelerator Technology:
- High-field, high-quality superconducting magnets
- High-power radio-frequency systems
- Ultrahigh vacuum systems
- Advanced accelerator designs
- Accelerator/spallation source applications
- Insertion device development: wigglers and undulators
- High-power, short-pulse lasers

Medical Technologies:
- Biomedical applications of nuclear technology
- Development and production of radio-nuclides/radiopharmaceuticals
- Development of particle and X-ray radiation therapies for cancer
- Medical imaging
- X-ray microbeam therapy

Biotechnology:
- Neutron and synchrotron x-ray scattering
- Large scale genome sequencing
- High resolution scanning and cryogenic electron microscopy
- Cloning, expressing and engineering genes
- Metal cluster compounds for electron microscope labels
- Phage displays for probing specific interactions
- Biocatalytic treatment of heavy oils

Environmental and Conservation Technologies:
- Ultra sensitive detection and characterization
- Environmental remediation and mitigation
- Waste treatment
- Disposal of nuclear materials
- Energy-efficiency technologies
- Fuel cell technologies
- Infrastructure modernization
- Transportation: Intelligent transportation systems, MAGLEV, RAPTOR
- Radiation protection
- Bioremediation technologies

Safety, Safeguards, and Risk Assessment:
- Safeguards, non-proliferation and arms control
- Design and development of non-proliferation reactors and fuel cycles
- Material and component survivability testing
- Remote sensing of chemical signatures
- Technical support for U. S. policy
- Safety analysis of complex systems
- Probabilistic risk assessment and management
- Human factors
- Energy-system modeling
- Structural, thermal hydraulics and nuclear design
- Integrated Safety Management

The following is a list of themes that are derived from the breadth and expertise expressed in Tables 1 and 2. The number of LDRD projects as related to these BNL themes is shown in Table 3.

Table 3 - THEMES

THEMES	Number of LDRD Projects
1 Scientific Facilities Operations • RHIC • AGS • NSLS • ATF • LEAF • STEM • Tandem • BMRR	1
2 Nuclear Physics • Quark/gluon plasma • Spin Physics	2
3 High Energy Physics • Standard Model • Rare Particles & Processes	1
4 Advanced Accelerator & Detector Concept and Designs - Advanced Instrumentation • Muon Collider • DUV-FEL • LHC • SNS	15
5 The Physics & Chemistry of Materials • Superconductivity • Magnetism • Surfaces • Nanostructure	6
6 Energy Sciences • Combustion • Catalysis • Bio-fuels • Batteries • Geothermal • Buildings	1
7 Environmental Sciences • Atmospheric • Terrestrial • Bio-remedial • Waste Technologies	3
8 Medical and Imaging Sciences & Technology	5
9 Advanced Computation	9
10 Biological Sciences	6
11 Critical Infrastructure	11
Totals	**60***

*The total number is greater than the number of LDRD projects since some projects come under more than one theme.

Overall, the LDRD portfolio supports all of the BNL themes and strategic objectives which in turn supports the DOE strategic initiatives.

Summary of Metric Data

Statistical data is collected on all projects for the annual report. Since LDRD is intending to promote high risk research, the data collected has nominal value on a project-by-project basis. It does provide a general overall picture of the LDRD Program productivity.

Some of the more common indicators/ measures of success are: 1) the number of proposed, received and approved projects, 2) amount of follow-on funding, 3) the number of patents applied for, and 4) the number of full-length papers published in other journals or publications.

Historically, statistics on the number of projects approved, compared to those rejected, show an overall approval rate of about 30 percent for new starts. Eight scientific departments were represented in the FY 2000 LDRD Program. From inception of the program through September 2000 (for FY 2000), 831 project proposals were considered and 265 were approved. These show and demonstrate that the LDRD Program at BNL is expanding and is generating interest from across the entire Laboratory population.

In FY 2000, the BNL LDRD Program funded 45 projects, 21 of which were new starts, at a total cost of $5,533,772. Included in this report is the Project Funding Table which lists all of the FY 2000 funded projects and gives a history of funding for each by year.

FISCAL YEAR	AUTH K$	COSTED K$	NO. REC'D	NEW STARTS
1985	1,842	1,819	39	13
1986	2,552	2,515	22	15
1987	1,451	1,443	29	8
1988	1,545	1,510	46	14
1989	2,676	2,666	42	21
1990	2,008	1,941	47	9
1991	1,353	1,321	23	14
1992	1,892	1,865	30	14
1993	2,073	2,006	35	14
1994	2,334	2,323	44	15
1995	2,486	2,478	46	13
1996	3,500	3,050	47	17
1997	4,500	3,459	71	10
1998	4,000	2,564	53	4
1999	4,612	4,526	67	25
2000	6,000	5,534	93	21
2001	6,000	----	97	38
TOTALS	50,046	41,068	831	265

An analysis of the FY 2000 projects shows that sixteen (16) of the projects were reported to have submitted proposals for grants or follow-on funding (several received funding), and forty-four (44) articles or reports were reported to be in publication or submitted for publication. Several of these projects have already experienced varying degrees of success, as indicated in the individual Project Program Summaries that follow. The complete summary of success indicators is as follows:

Follow-on Activity of LDRD Projects	
	Number of <u>Projects</u>
Informal Publications	**62**
Formal Papers	**44**
Grants/Proposals/Follow-on Funding	**16**
Patents	**2**

In conclusion, the overall LDRD Program has been successful. In FY 2000 the LDRD Program has increased significantly at BNL. This increase in size is in direct relation to the Laboratory's Management identifying the LDRD Program as an important part of its future. The LDRD Program is a key component for developing new areas of science for the Laboratory. In FY 2000 alone the Laboratory has experienced a significant scientific gain by the achievements of the LDRD projects.

APPROVED LABORATORY DIRECTED RESEARCH AND DEVELOPMENT
FY 2000 PROJECTS FUNDING TABLE

						Actual Cost		Budget	Requested	
									Not Committed	
Proj No	PROJECT TITLE	P. I.	Dept.	Theme	FY 98	FY 99	FY 00	FY 01	FY 02	Total
98-23A	Performance Enhancement in a Photoinjector Electron Linac	E.Johnson	NSLS/725D	4		301,000	266,298	252,000		819,298
98-23B	Pulse Compression and Emittance Preservation in a High Brightness Electron Linac	W. Graves	NSLS/725D	4		150,000	133,000	131,000		414,000
99-01	Ultra-fast Detector based on Optical Techniques	Y. Semertzidis	PHYS/510A	4		113,300	88,932	80,000		282,232
99-03	NOVA: Networked Object-Based enVironment for Analysis	T. Wenaus	PHYS/510A	9		99,900	31,990			131,890
99-05	Aerosol Module for Climate Models Using Advanced Computer Techniques	C. Benkovitz	Env. Sci./815E	7		98,900	78,475			177,375
99-06	Environmental Carbon Observatory (ECO)	G. Hendrey	Env. Sci./815E	7		346,900	240,000			586,900
99-10A	Parallel Algorithms for Accelerator Design	J. Glimm	Env. Sci./515	9		125,805	170,000			295,805
99-10B	Photonic Band Gaps in Nanostructured Materials	J. Davenport	Env. Sci./515	5, 9		95,000	140,000			235,000
99-10C	Parallel Algorithms for Biomedical Image Processing	J. Davenport	Env. Sci./515	8		125,000	180,000			305,000
99-26	Electron Diffraction Studies of Charge Ordering in Transition-Metal Oxides	Y. Zhu	Env. Sci/480	5		86,800	74,696			161,496
99-28	Evaluation of a Millimeter Quasi-optical Source for Non-destructive Detection & Analysis	M. Ruckman	ES&T/703	4		84,800	59,852			144,652
99-40	Microdistribution Studies of Boron 10 for Boron Neutron Capture Therapy Using Transmission Electron Microscopy	R. Ma	MED/490	8		117,600	58,867			176,467
99-41	Efficasy of Unidirectional Microbeam Radiation Therapy in Treating Malignant Tumors: Preclinical Studies in Rats and Mice	A. Dilmanian	MED/490	8		119,600	149,204	126,000		394,804
99-45	Toxin Bio-Information Resource	S. Swaminathan	BIO/463	4, 10		74,900	75,760			150,660
99-46	Experimental and Theoretical Investigation of Transition Metal Oxides	J. Hill	PHYS/510B	5		84,400	61,969	60,000		206,369
99-48	Pulsed laser Deposition Facility	P. Johnson	PHYS/510B	4, 5		122,300	57,300			179,600
99-50	Ultrashort bunch length Monitor	W. Graves	NSLS/725D	4		110,200	65,274			175,474
99-51A	High Gain FEL Amplifier	G. Rakowsky	NSLS/725D	4		100,000	100,000	184,000		384,000
99-51B	Deep Ultra-Violet Free Electron Laser Optimization	E. Johnson	NSLS/725D	4		396,900	298,107	184,000		879,007
99-53	Development of High Brightness Electron Sources	I. Ben-Zvi	NSLS/725C	4		201,400	199,807	100,000		501,207
99-56	Attosecond Pulse Generation in High Harmonics	L. DiMauro	CHEM/555A	4		109,300	77,988	75,000		262,288
99-57	Development of a 2-D Ion Imaging Detector for VUV-FEL Applications	M. White	CHEM/555A	4		98,800	78,291			177,091
99-59	Application of Quantitative MRI: Water Content and Blood-Brain-Barrier Permeability in Multiple Sclerosis	W. Rooney	CHEM/555A	8		74,400	70,272			144,672
99-62	In-Situ Time-Resolved Studies of Catalysts for SOx and NOx Decompostion using Synchrotron Radiation"	J. Rodriguez	CHEM/555A	6		122,000	48,789	60,000		230,789

APPROVED LABORATORY DIRECTED RESEARCH AND DEVELOPMENT
FY 2000 PROJECTS FUNDING TABLE

						Actual Cost		Budget	Requested	
									Not Committed	
Proj No	PROJECT TITLE	P. I.	Dept.	Theme	FY 98	FY 99	FY 00	FY 01	FY 02	Total
00-05A	Exploration of the Object Oriented Approach to Reconstruction Algorithms	H. Gordon	PHY/510A	9			100,000			100,000
00-05B	Assessment of GEANT4 as a Model for the ATLAS Liquid Argon Calorimeter Test Beam Data	H. Gordon	PHY/510A	4, 9			105,283			105,283
00-06	Probing extreme QCD: articulating the physics goals of an electron-relativistic heavy ion collider (eRHIC) at BNL	R. Venugopalan	PHY/510a	2			83,928	85,000	85,000	253,928
00-25	Novel Techniques to Measure Aerosols and aerosol Precursors	S. E. Schwartz	Env. Sci./815E	7			149,474	242,000	242,000	633,474
00-27	Nanocomposites of Silicon Polymorphs and Related Semiconductor Systems	D. O. Welch	Env. Sci./480	5			79,117	70,000	70,000	219,117
00-28	Preparations for Finalizing MATAC Installation	L. Wielopolski	Env. Sci./490D	1			58,480			58,480
00-32	Microvascular Endothelial Cells as Targets for Ionizing Radiation: In Vitro and In Vivo Models	L. Pena	MED/490	8			82,633	100,000		182,633
00-35	Investigationg Service Chemical Reactions and Kinetics for Atomic to the Nano Scale	J. Hrbek/J. Larese	CHEM/555A	5			48,849			48,849
00-40	The Structure of Membrane Proteins: Monolayers and Thin Films	B. Ocko	PHY/510A	10			16,566	50,400	50,400	117,366
00-42A	Mobile Agent Based Monitoring of Distributed Computing Systems	R. Ibbotson	C-A/510C	9			144,871			144,871
00-42B	Demonstration of Advanced Commercial Ethernet Technology	T. Healy	ITD/515	9			100,000			100,000
00-42C	Cyber Security for Wide Area Distributed Collaborations	S. Misawa	PHYS/510C	11			100,000			100,000
00-42D	Data Mining Strategies for HENP Experiments	B. Gibbard	PHYS/510C	2, 3, 9			100,000			100,000
00-42E	Parallel Linux System	T. Throwe	PHYS/510C	9			100,000			100,000
00-43	Understanding the Pathways of Ubiquitin Dependent Proteolysis	M. Bewley	BIO/463	10			244,247	215,000	215,000	674,247
00-44	Structural Characterization of DNA-PK, A Human DNA Double-Strand	J. M. Flanagan	BIO/463	10			44,132	95,200		139,332
00-45	New Protein Expression Tools for Proteomics	P. L. Freimuth	BIO/463	10			41,698	111,000	111,000	263,698
00-47	High-throughput Structure Determination of the Human Proteome Project	F. W. Studier	BIO/463	10			575,570	290,000	290,000	1,155,570
00-49	Design Study of a Solid Target for Spallation Neutron Sources	J. Hastings	NSLS/725D	4			301,241	194,000	194,000	689,241
00-61	Remote Full-Field Optical Measurement of Structural Intergrity	R. Hall	ES&T/139	11			58,000			58,000
00-93	Muon Collider and Storage Ring Neutrino Beam Study	R. Palmer	PHY/901A	4			194,812			194,812
			Total				5,533,772	2,704,600	1,257,400	12,854,977

LABORATORY DIRECTED RESEARCH AND DEVELOPMENT

2000 PROJECT PROGRAM SUMMARIES

Performance Enhancement in a Photoinjector Electron Linac

Erik D. Johnson 98-23A
Louis F. DiMauro
William S. Graves
Brian Sheehy and
Xijie Wang

PURPOSE:

This project explores previously unmapped parameter space in Photoinjector Electron Linacs with the goal of finding approaches to dramatically improve the performance of this class of machines. There are conflicting theoretical predictions of performance particularly when short and shaped laser pulses are used for driving the photocathode. Some project dramatic enhancement, some marginal improvement, and at present no data exist to sort them out. At a minimum this project represents an experimental investigation to corroborate theory; if successful it provides a proof of principle for a significantly improved performance electron machine.

APPROACH:

In previous supported activities at BNL, the Accelerator Test Facility (ATF) developed an RF photocathode gun that was the starting model for our gun (Gun IV). Our gun can be run at higher repetition rate (due to enhanced cooling). To allow better control of the temporal characteristics of the light used to stimulate emission from the cathode, we have developed a laser system using Titanium Sapphire technology, which provides superior bandwidth to allow pulse shaping.

TECHNICAL PROGRESS AND RESULTS:

In FY 1999, we obtained approval for our Safety Assessment Document and Accelerator Safety Envelope to allow us to start commissioning and testing with photo-electron beam. The laser system and photo-injector have continued to evolve as the commissioning process proceeded.

In FY 2000, we had performed preliminary fault studies that have verified the shielding calculation predictions for low average current beam. When higher average current beam has been reliably established (~20 nA), final fault studies will be performed. Photo-beam has been produced and accelerated to the full energy (~200 MeV). Electron bunches of up to 0.3 nC have been accelerated to full energy with normalized emittance of 4 π mm-mrad. With further optimization of the laser and photoinjector operating techniques, we believe charge the order of 1 nC per bunch with comparable or improved emittance should be possible.

The enhancement of the overall performance of the linac is following an iterative route of comparison of experimental data with simulation. Evaluation and improvement of the mode quality and profile of the laser beam illuminating the photocathode is one focus area for improvement. The other major thrust is a continuing effort in simulation of the photoinjector properties to adjust operating performance of the linac. Variables under study include the field balance, operating RF power levels, laser to gun RF phase, gun to linac phase, and laser parameters at the cathode (spot size, pulse length and profile). Systematic study of these parameters will continue through FY2001.

SPECIFIC ACCOMPLISHMENTS:

This work was presented at the SPIE meeting in San Jose in January 2000, 'The Deep Ultra-Violet Free Electron Laser (DUV-FEL) at Brookhaven National Laboratory' E.D. Johnson, I. Ben-Zvi, L.F. DiMauro, W.S. Graves, R.N. Heese, S. Krinsky, J.C. Sutherland, X. Wang, L.-H. Yu, in Biomedical Applications of Free-Electron Lasers, SPIE Vol. 3925 (2000) 26.

An invited report on the project was also presented at the Lasers and Short Wavelength Applications (LSWave) 2000 Meeting (a Satellite of the Synchrotron Radiation Instrumentation Meeting) at TU Berlin August 26, 2000, 'Overview of US Single Pass FEL Projects' E.D. Johnson.

The approved Safety Assessment Document and Accelerator Safety Envelope for the experiment can be viewed at our website http://nslsweb.nsls.bnl.gov/nsls/org/SDL/ .

LDRD FUNDING:

FY 1999	$301,000
FY 2000	$266,298
FY 2001 (budgeted)	$252,000

Pulse Compression and Emittance Preservation in a High Brightness Linac

William S. Graves *98-23B*
Richard Heese
Erik D. Johnson

PURPOSE:

Free electron lasers will obtain substantial performance gains if peak current in electron linacs is increased. This can be achieved by compressing the length of the electron bunch, but it is only beneficial if other properties of the beam, such as emittance, are not degraded. Undesireable emittance growth due to space charge repulsion and the emission of coherent synchrotron radiation (CSR) is expected to limit the maximum peak current. Existing theories vary by more than an order of magnitude on the effect of CSR on emittance. By an experimental study, we can quantify its effect and investigate some of the proposed schemes to mitigate the emittance dilution induced by CSR. If successful, this project will help define the practical limits for the use of pulse compression in advanced machines.

APPROACH:

The peak current from a state-of-the-art photoinjector is limited to about 150 A due to space charge effects. We will increase this to as much as 1000 A by compressing the electron bunch after it has been accelerated to high energy.

A four magnet chicane has been installed at the Deep Ultra-Violet Free Electron Laser (DUVFEL) to compress the beam. The design of this compressor is optimized to reduce CSR emission while producing a short bunch. It has flexibility to alter the bend angle or drift distances between magnets to take advantage of experimental results. It also has the necessary diagnostics, including multiple bunch length measurement instruments and high precision emittance diagnostics, required to measure the effects of CSR on beam emittance.

The bunch length is compressed from approximately 5 ps to 0.2 ps. This process depends sensitively on the phase of the electron beam relative to the accelerating RF field. The phase must be measured and controlled with an accuracy of less than 1 ps. Our design includes instrumentation and controls for this purpose.

TECHNICAL PROGRESS AND RESULTS:

In FY 1999, studies were carried out using the accelerator design codes MAD and PARMELA to optimize the compressor and accelerator parameters. The bunch compressor and its associated diagnostics were built and installed. Work began on phase and amplitude detectors to measure and control the RF phase to the required precision.

In FY 2000, the RF phase detectors were completed, bench tested, and installed. Commissioning of the accelerator, Ti:Sapphire drive laser, emittance and bunch length diagnostics, and bunch compressor began. Initial beam measurements at the bunch compressor, and at the end of the linac were carried out and are shown in Tables 1 and 2.

The emittance diagnostics, consisting of YAG:Ce scintillators, CCD cameras, quadrupole magnets, and software controls were installed and are fully operational.

Table 1

Beam Parameters at Bunch Compressor	
Energy	82 MeV
Energy spread	0.2%
Bunch length	2.0 – 3.0 ps
Charge	0.1 nC
Emittance	4 – 8 mm-mrad
Timing stability	0.5 – 3 ps

Table 2

Beam Parameters at Linac End	
Energy	200 MeV
Energy spread	0.07%
Bunch length	0.2 – 3.0 ps
Charge	0.1 nC
Emittance	4 – 8 mm-mrad
Timing stability	0.5 – 3 ps

There are several devices to measure short electron pulses: a liquid helium cooled bolometer to measure the far infrared CSR spectrum, a high resolution visible light spectrometer to measure single shot undulator radiation spectra, and an electron beam dispersion section with YAG:Ce scintillator that uses the linac itself as a bunch length diagnostic in a technique known as RF-zero phasing. The bolometer and single-shot spectrometer were received and bench tested, and are currently being installed.

Initial bunch compression studies were carried out using the RF-zero phasing technique. Images from the measurements and profiles of the beam current are shown in Figures 1 – 4.

In FY 2001, commissioning of the accelerator will continue with an emphasis on increasing the amount of charge and reducing the observed timing jitter. The remaining bunch length diagnostics will be made operational and detailed studies of the effects of CSR emission on the beam's emittance will begin.

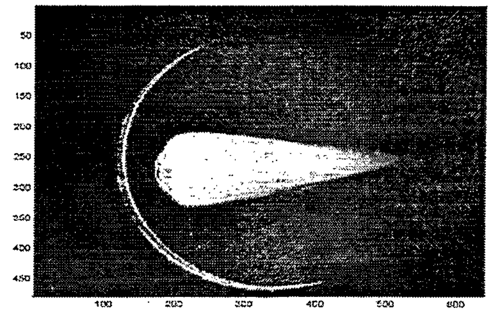


Figure 1: Image of uncompressed beam on YAG:Ce scintillator.

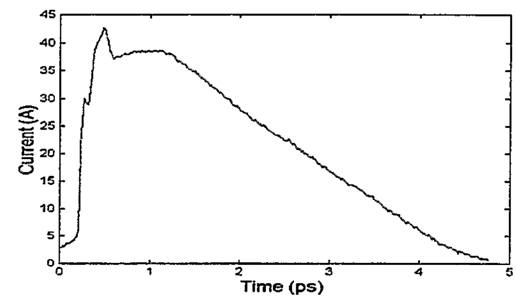


Figure 2: Current profile of uncompressed beam showing 3 ps bunch length and 40 A peak current.

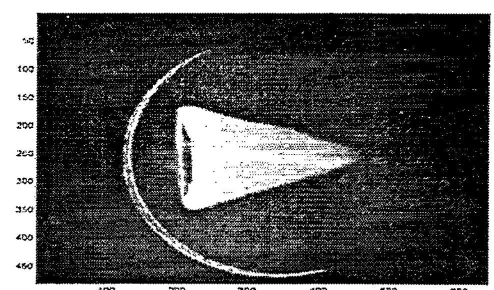


Figure 3: Image of compressed beam on YAG:Ce scintillator.

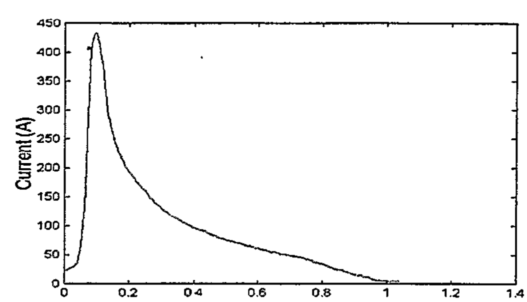


Figure 4: Profile showing 0.2 ps bunch length and 425 A peak current of compressed bunch.

SPECIFIC ACCOMPLISHMENTS:

In recognition of our effort to produce and measure ultrashort electron bunches, BNL was asked to organize and host the "LCLS Fast Instrumentation Workshop", held on March 3,4 2000 with 26 attendees from 8 institutions. SLAC also provided $30k funding for R&D to develop this instrumentation. Several talks were based on work developed under this LDRD project including:

Measurement Methods and Solutions for Ultrashort Bunches, W.S. Graves, presented at the above workshop.

Bunch Length Measurements using a Laser Time Gate, W.S. Graves, presented at the above workshop.

LDRD FUNDING:

FY 1999	$151,000
FY 2000	$134,000
FY 2001 (budgeted)	$131,000

Ultra-Fast Detector Based on Optical Techniques

Yannis K. Semertzidis *99-01*

PURPOSE:

A charged particle beam detector based entirely on electro-optical (E-O) techniques is a very promising way to reach time resolution in the range of 10^{-11} s (10ps) to 10^{-14} s (10fs) in a non-destructive way. Efforts are underway at accelerators around the world, including the accelerator test facility (ATF) at BNL, to produce beams with ultra-short bunch lengths and can benefit greatly with the development of this diagnostic technique.

APPROACH:

During the last decade there has been a revolution in sensing ultra-fast electric fields with unprecedented time resolution. Our expertise with optical techniques together with our particle and accelerator physics background helped us marry the two fields. There are 3 collaborating institutes and 10 physicists participating in the effort: V. Castillo, R. Larsen, D.M. Lazarus, D. Nikas, C. Ozben, Y.K. Semertzidis, T. Srinivasan-Rao, and T. Tsang from BNL; L. Kowalski from Montclair State University; and D.E. Kraus from University of Pittsburgh.

The electric field from a relativistic charged particle beam is Lorentz contracted and forms a transverse E-field front. The amplitude of this E-field is proportional to the amount of charge present in the beam. Therefore, a transverse electric field sensor with a good time resolution compared to the time duration of the beam, can reveal the longitudinal profile of the beam. We proposed to use crystals as the transverse E-field sensors by means of the E-O effect.

After we observed the first signals there were still questions about their source. The electric fields present near charged particle beams are very small, and the backgrounds due to wake fields provide significant competition. In order to study this we have constructed an ellipsometer which consists of a polarizer to polarize the laser beam, an electro-optic crystal ($LiNbO_3$), a Quarter Wave Plate (QWP), and an analyzer (i.e. polarizer set in almost full extinction mode). In the absence of an electric field the laser beam going through the crystal is linearly polarized when it enters the crystal and linearly polarized when it exits it. If there is an electric field present near the crystal, then the crystal becomes birefringent and the exiting laser light becomes elliptically polarized for the time the electric field is present. The QWP transforms this ellipticity into a rotation. The analyzer turns the rotation into a time dependent light amplitude modulation. This ellipticity from the $LiNbO_3$ crystal is proportional to the electric field present near the crystal and the E-O effect in this case is called the Pockel's effect. For other materials the induced ellipticity is proportional to the square of the electric field in which case the E-O effect is called the Kerr effect. We have chosen to use the Pockel's effect since it dominates in the small electric field region.

TECHNICAL PROGRESS AND RESULTS:

Our group made the first observation in the world of a charged particle beam by means of the E-O effect. The sensor we used was a commercially available E-O crystal placed near the 10-15ps electron beam available at the ATF of BNL. The total charge per bunch was about 0.6nC and the repetition rate 1.5Hz. This crystal formed a wave-guide for the laser light, and it was enclosed in a metal case. We had to modify the metal case around the crystal in order to gain beam access to it.

In FY2000, we assembled a system using a bulk crystal ("free space setup") bringing the laser light by means of a fiber all the way from the control room to the beam-line. The laser light came out from the fiber and was coupled into the crystal which was located in the vacuum chamber of the beam-line with the matching optics. After the crystal, the laser light traversed the QWP, and then was coupled to another fiber which carried it to the control room where it was detected by a fast photodiode following the analyzer. The output of the amplifier was connected to a fast oscilloscope.

We again observed the signal in the presence of the charged particle beam. The observed rise-time of the signal was 70ps limited by the bandwidth of the oscilloscope. In a series of tests we checked the polarity dependence of the signal when the beam was above versus below the crystal. The electric field sensed by the crystal changes polarity and so did the signal. We also rotated the laser polarization vector by 90 degrees and again the signal polarity flipped sign as expected. Due to the Lorentz contraction and the finite speed of light, the signal dependence is inversely proportional to the distance from the crystal. The 1/r dependence was confirmed in a series of measurements.

This method is fully utilized when all parts of the system have very high bandwidth, and there are no slow components in it. One way to achieve this is to use only components based on E-O effects. In place of the charge pre-amplifier we will use (in the next step) a streak camera capable of bringing the time resolution to below 10ps. In the laboratory we have tested the operation mode of a streak camera available to us, and we were able to achieve the above time resolution with a low energy pulsed laser in the presence of a Continuous Wave (CW) laser used to simulate the background. In FY2001, we will achieve the signal detection using electric fields between parallel plates. The output of this setup is coupled to a streak camera which has a time resolution of 2-10ps. After this is achieved we will run at the ATF with the electron beam providing the electric field near the crystal.

After this program is completed we will use Frequency Resolved Optical Gating (FROG) techniques or new techniques developed by our group to achieve sub-ps time resolution in single shot. We are currently seeking funding from DOE for the application of FROG or our new techniques.

SPECIFIC ACCOMPLISHMENTS:

We are in the process of applying for a patent on our method of achieving sub-ps time resolution.

We have made the following presentations (with proceedings available):
Y. Semertzidis, et al., Particle Accelerator Conference, NY, March 29, 1999.
D. Lazarus et al., International Europhysics Conference-HEP99, Tampere, Finland, 1999.
D. Nikas, et al., DPF2000, Columbus Ohio, August, 2000.
We published the article (refereed): Y.K. Semertzidis, et al., NIMA 396, 452, 2000.
Submitted the following article (refereed): T. Tsang, et al., JAP.

LDRD FUNDING:

FY 1999	$113,345
FY 2000	$ 88,932
FY 2001 (budgeted)	$ 80,000

NOVA: Networked Object-based enVironment for Analysis

Torre Wenaus 99-03
Tim Hallman
Pavel Nevski
Sasha Vanyashin

PURPOSE:

Emerging computational grid infrastructure opens promising directions of research in data management for high throughput distributed computing. Our goal has been to build a generic coordinating framework for distributed analysis that can be widely applied within and beyond High Energy and Nuclear Physics (HENP). The project pioneered novel approaches based on resilient data management algorithms emphasizing fault tolerance.

APPROACH:

Computing in HENP experiments has historically been centralized. The NOVA project envisioned a coming era of distributed grid computing and initiated new developments in that area. Feasibility of grid computing in HENP experiments relies heavily on data management solutions. Traditional object-oriented techniques encapsulating data and algorithms are difficult to scale to the multi-petabyte data volumes expected from a new generation of HENP experiments at the Relativistic Heavy Ion Collider (RHIC) and Larger Hadron Collider (LHC). The NOVA project investigates scalability of novel computing paradigms like "agent" computing or generic computing that separate algorithms from data.

We designed a novel meta-level architecture comprised of the four domains: mobile analysis client, central analysis server, middleware, and data management. A mobile analysis client interacts with a central analysis server and associated monitoring and control tools via web-based middleware to support analysis in a distributed heterogeneous environment. The client is integrated with software distribution, management and version coordination tools to meet the collaborative analysis needs of a widely distributed community. Central data and file catalogues with associated tools for controlling and monitoring data locality, data browsing, and data model evolution for data intensive analysis are included. NOVA was developed using an iterative process driven by user participation and closely coupled to prototyping in real-world experiments.

In selecting technologies we imposed the requirements that they should be free or nearly so to minimize buy-in cost. We have adopted many open software tools including the MySQL database, the Apache web server and associated integrated tools, and the ROOT object-oriented toolkit for HENP analysis. Our reliance on Internet driven open software technologies differs substantially from the in-house or commercially developed solutions current in the field, but offers large benefits in exploiting this area's exponential growth.

TECHNICAL PROGRESS & RESULTS:

In FY 2000, we have completed the implementation of all components of the architecture, guided by application and prototyping experience in experiments. Because NOVA developers are the Solenoidal Tracker at RHIC (STAR) and A Toriodal Lhc ApparatuS (ATLAS) collaborators, these experiments have served as convenient test beds, but the tools themselves are generic; we have established NOVA as an experiment-independent tool set for distributed analysis. The component-based approach pioneered in NOVA has generated interest within current Grid projects.

We have performed scalability testing with management of multi-terabyte data sets and large-scale analysis. Data sets from the STAR experiment that have been used in the test are shown below.

Multi-Terabyte Data Set Management

Data Set Description	*Size, TB*
Detector readout structures	11
Simulated readout structures	12
Simulated reconstructed objects	6
Reconstructed structures	8
Reconstructed objects	2

The project developed novel approaches for the high throughput computing – another core element for emerging computational grids. Independent event processing in HENP is well suited for computing in parallel. NOVA prototypes exploited inexpensive mass market components by providing fault tolerant resilience (instead of expensive total system reliability) via highly scalable management tools. Robust data management is required since a large amount of data has to be moved to each node before and/or saved after each job. The architecture of NOVA's active object coordination framework implements a multi-level hierarchical agent model. It provides fault tolerance by splitting a large overall task into independent atomic processes, performed by lower level agents, with necessary control functions performed by higher level agents managing distributed data caches. The system has been tested in production environments for STAR simulation. NOVA architecture controlled processes on more than a hundred processors at a time and has run for extended periods of time. Five terabytes of simulated data have been produced.

The generic nature of the NOVA two-level architecture solution for fault tolerance in distributed environments has been demonstrated by its successful test for grid file replication services at a coast-to-coast scale between BNL and LBNL.

SPECIFIC ACCOMPLISHMENTS:

NOVA FY2000 results were presented to the HENP community at the Second International Conference on Modern Trends in Computational Physics in July 2000 and at the Computing in High Energy Physics conference CHEP2000 in February 2000. A NOVA paper is published in the proceedings. In FY2000, presentations on NOVA have been made to the Particle Physics Data Grid collaboration, Center for Data Intensive Computing, and to the wider community at the High Performance Networking and Computing Conference "SC99." The NOVA project is presented on the World Wide Web at http://www.usatlas.bnl.gov/computing/nova. As a direct result of NOVA, funding from LBNL's HENP Grand Challenge project was obtained to support one of us (Sasha Vanyashin) in FY2000 to integrate Grand Challenge software with STAR software incorporating NOVA components. The project has established a recognized distributed analysis expertise at BNL that has led to expected US ATLAS Computing Project funding for BNL in this area in the next year.

Concluding talks at the CHEP2000 conference emphasized "the Dream" of HENP physics analysis – transparent user access to all data in the event. Deployment of NOVA project components together with the Grand Challenge software provides transparent user access to all data stored on mass store (tape) as well as disk, in a production environment – "the Dream" is coming true.

LDRD FUNDING:

FY 1999	$99,894
FY 2000	$31,990

Aerosol Module for Climate Models Using Advanced Computer Techniques

C. M. Benkovitz — *99-05*
S. E. Schwartz

PURPOSE:

To develop and apply advanced computational techniques that will allow the inclusion of aerosol transport and evolution processes in global climate models and regional scale air quality models. This modeling capability will permit accurate evaluation of the influences of anthropogenic aerosols on climate and development of effective and efficient strategies for control of regional scale aerosol air quality.

APPROACH:

Background. Atmospheric aerosols contribute to climate change by modifying radiation and modifying the properties of clouds. It is, therefore, necessary to represent these aerosol influences in climate models. Because aerosols are highly variable in the atmosphere (spatially, temporally, and in their microphysical properties) and because this variability is correlated with other atmospheric properties such as cloudiness and humidity, it is necessary to represent aerosols dynamically in climate models instead of using some static average aerosol field. In particular it is necessary to represent aerosol microphysical properties (key is size distribution) that govern aerosol radiative influences. Present techniques that attempt to achieve this by modeling the full- size distribution place enormous demands on computational resources and are thus impossible to incorporate into global climate models.

Scope. This work focuses on developing efficient means of representing aerosol chemical and microphysical processes in chemical transport models by developing and testing moment-based representation of aerosol size distribution, and by developing and testing parallelized computer codes for representing these processes.

Methods. Moment-based representation of aerosol properties and evolution was through the Quadrature Method of Moments, developed in previous work at Brookhaven. This project examined the feasibility of incorporating this approach in large-scale chemical transport models.

The parallelization used a virtual Cartesian application topology. The physical domain of the chemical transport model was partitioned into multi-block grids, which were then mapped onto individual processors. The partition of the whole three-dimensional region of space into individual subdomains leads to computational units of smaller size, which are to a large extent independent of each other. As a result, the computation can be performed in parallel, thus reducing the overall wall-clock time to perform a simulation. The longitudinal grid partitioning approach takes advantage of the facts that the number of grid points of the model in the longitudinal direction is much greater than those of the other directions, and that the vectorization performance would be maintained under this partitioning due to the storage order of array elements. The longitudinal grid partitioning approach also creates a work-intensive coarse-grained parallelism which takes better advantage of powerful processors, such as those of today's distributed memory supercomputers and those of a workstation cluster.

Other BNL participants were Hong Ma, Robert McGraw, Douglas Wright, James

Davenport, and Arnold Peskin provided advice. External collaborations were with Daniel Rosner (Yale) and Prasad Kasibhatla (Duke).

TECHNICAL PROGRESS AND RESULTS:

In FY 1999, we demonstrated the ability to represent aerosol microphysics in a sub-hemispheric scale transport and transformation model by the method of moments and established the ability to accurately compute aerosol optical and radiative properties from the moments of the size distribution, thereby substantiating the utility of the moment approach for examining the influence of aerosols on climate. We made substantial progress in parallelizing a sub-hemispheric chemical transport and transformation code. This will serve as a host model for parallelized aerosol code.

Parallelization of the chemical transport code was brought to conclusion in FY 2000. With 120 Cray T3E nodes, the parallel code only uses about 12 s per simulation hour (down from 6.5 CPU min on a SUN Enterprise 4500), an improvement by a factor of about 30. This improvement makes feasible model "experiments" (runs with changed model inputs) that would otherwise not be possible, and as well gives credence to the ability to include representation of aerosols in climate models.

Major new findings with respect to representation of aerosol processes by moment methods are: 1) It is possible to accurately represent the partitioning of aerosols into activated and non-activated components using moment methods, specifically the "MIDAS" (Multiple Isomomental Distribution Aerosol Surrogate) method developed in this project; this partitioning is a strenuous challenge because the "step function" is not well represented by low-order polynomials, 2) The quadrature method of moments is stunningly successful in representing bivariate aerosol distributions. The approach was tested on modeling the dynamics of a population of inorganic nanoparticles undergoing simultaneous coagulation and particle sintering in flames. For evaluation purposes, and to demonstrate the computational efficiency of the bivariate QMOM, benchmark calculations were carried out using a high-resolution discrete method to evolve the particle distribution function for short to intermediate times. Time evolution of a selected set of 36 low-order mixed moments was obtained by integration of the full bivariate distribution and compared with the corresponding moments obtained directly using the QMOM. Errors of less than 1% were obtained over substantial aerosol evolution, while requiring only a few minutes (rather than days) of CPU time.

SPECIFIC ACCOMPLISHMENTS:

Refereed Publications

FY 1999

Wright, D.L.; McGraw, R.; Benkovitz, C. M.; and Schwartz, S.E. Six-moment representation of multiple aerosol populations in a sub-hemispheric chemical transformation model. *Geophys Res. Lett.* **27**, 967-970 (2000).

Wright, D.L. Retrieval of optical properties of atmospheric aerosols from moments of the particle size distribution. *J. Aerosol Sci.* **31**, 1-18, 2000.

FY 2000

Wright, D.L.; McGraw, R.; and Rosner, D.E., Bivariate extension of the quadrature method of moments for modeling simultaneous coagulation and sintering of particle populations, *J. Coll. Interface Sci.*, submitted, 2000.

Wright, D.L.; Kasibhatla, P.S.; McGraw, R.; and Schwartz, S.E. Description and evaluation of a six-moment aerosol microphysical module for use in atmospheric chemical transport models. *J. Geophys. Res.*, submitted, 2000.

McGraw, R.; Wright, D.L.; Benkovitz, C.M.; and Schwartz, S.E. From aerosol microphysics to geophysics using the method of moments. In *Proceedings of the 15th International Conference on Nucleation and Atmospheric* Aerosols, Editors Hale, B.N.; and Kulmala, M. (AIP, 2000) pp 785-788.

Meeting/Conference Presentations.

FY 1999

Benkovitz, C.M. Preparing to Model the ACE Experimental Periods with GChM-O Version 2 and Recent Developments Regarding Aerosol-Related Emissions Inventories. Third Annual Workshop of the Northern Aerosol Regional Climate Modelling Project (NARCM), March 1-2, 1999, Toronto, Ontario, Canada.

Benkovitz, C.M.; Schwartz, S.E.; Mubaraki, M.A.; Miller, M.A.; and Bates, T.S. Simulating Sulfur for the ACE-2 Experiment: Preliminary Results. Presented at the Sixth Scientific Conference of the International Global Atmospheric Chemistry Project (IGAC) Bologna, Italy, September 13-17, 1999.

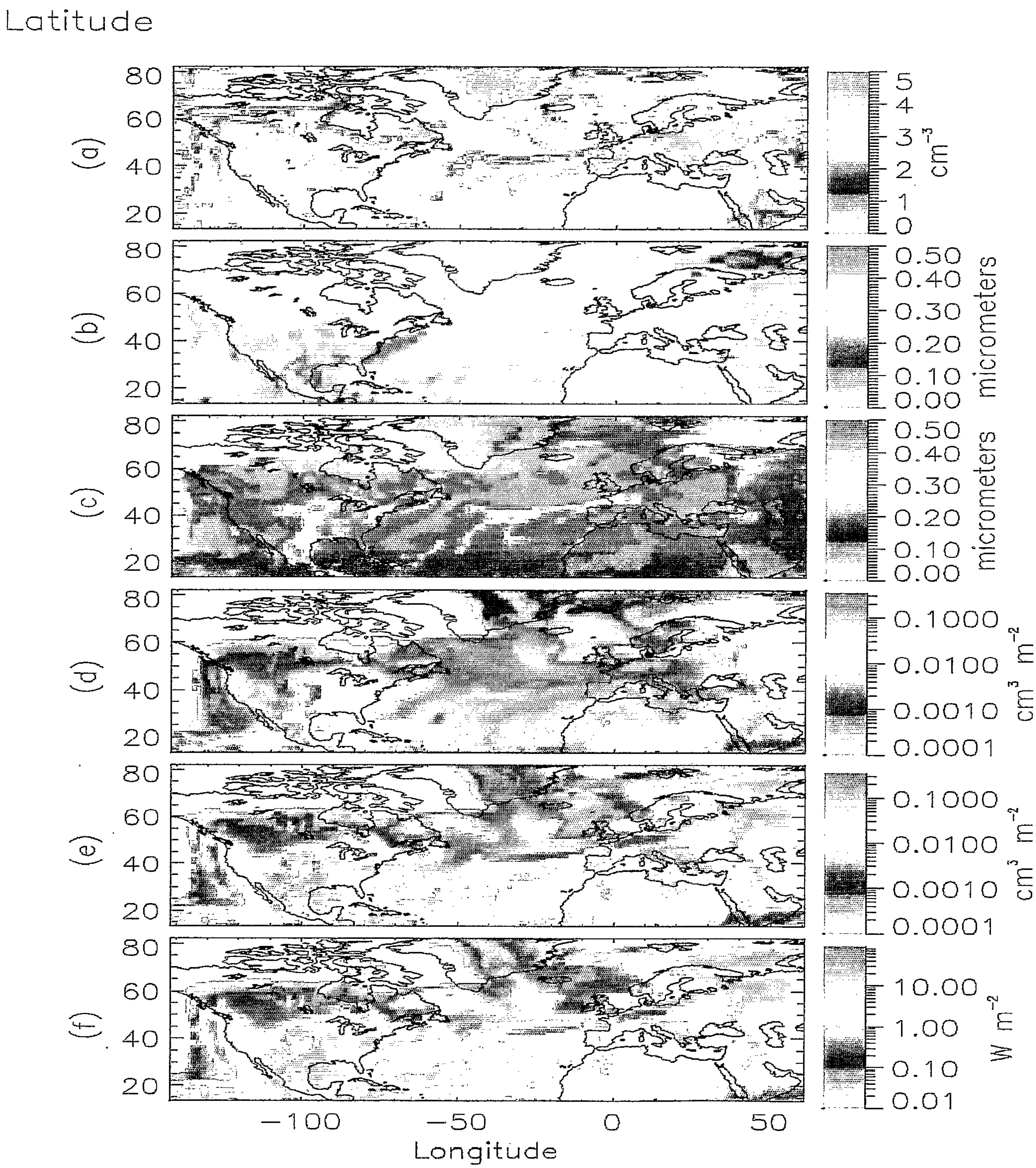
Wright, D.L.; McGraw, R.L.; Benkovitz, C.M.; and Schwartz, S.E. Aerosol Dynamics and Shortwave Radiative Forcing in a Sub-hemispheric Model by the Method of Moments. American Geophysical Union 1999 Spring Meeting, Boston, MA, Jun 1-4, 1999; paper A22G-08. Abstract: *Eos, Trans. Amer. Geophys. Un.* **80** (No. 17, Supplement) S41 (1999).

FY 2000

McGraw, R.; Wright, D.L.; Benkovitz, C.M.; and Schwartz, S.E. Moment representation of aerosols in a sub-hemispheric chemical transport model, Presented by R. McGraw at the 4th NARCM (Northern Aerosol Regional Climatological Model) Workshop, Toronto, Ontario, Canada, March 1-2, 2000. Invited Presentation.

LDRD FUNDING:

FY 1999	$98,887
FY 2000	$78,475



Output of subhemispheric-scale chemical transport model using moment-based representation of aerosol properties; properties of sulfate aerosol are derived from the evolved moments of the size distribution for October 22, 1986, 0600 UT. (a) $\log_{10}$ number concentration (μ_0) at 32 meters, (b) number mean radius ($r_{ave} = \mu_1/\mu_0$) at 32 meters, (c) effective radius ($r_{eff} = \mu_3/\mu_2$) at 32 meters, (d) column integral of condensed aerosol volume for the dry aerosol, (e) column integral of condensed aerosol volume for the aerosol at the ambient relative humidity, and (f) magnitude of the change in top-of-atmosphere radiative flux at wavelength 550 nm. White regions indicate values below the plotting scale. From Wright *et al.* (2000).

Environmental Carbon Observatory (ECO)

George R. Hendrey *99-06*

PURPOSE:

The purpose of the ECO LDRD project was to increase scientific and technical capabilities at BNL for research in topics relating to global climate change. The goal was to put in place a coherent system for integrating environmental carbon cycle measurements and models and demonstrate their integration and utility.

APPROACH:

Background-- Quantifying exchanges of water and CO2 between the terrestrial biosphere and the atmosphere and understanding processes regulating these exchanges are critical to assessing the potential for future anthropogenic climate changes. OBER has established programs to address these issues. The "AmeriFLux" program aims to quantify the contemporary flux of CO2 and water between the terrestrial biosphere and the atmosphere by measuring the covariance of the scalar values and wind vector variables at numerous research sites in North America. The free-air CO2 enrichment (FACE) program, in which BNL plays a leading role, seeks to describe the responses of plants and ecosystems to future elevation of CO2 in the atmosphere. The means for relating measurements made in FACE to regional contexts is lacking, and the AmeriFlux network is seen as potentially providing a framework for that scaling.

Scope-- ECO aimed to develop tools and capabilities at BNL that could help to address two topic areas: spatial scaling of point- or plot-based field data and the need for a general framework for ecosystem modeling. For the first topic the idea developed in the ECO LDRD was that an expanded AmeriFLux network would allow explicit estimates of spatial variability in carbon flux for a region. The ECO LDRD sought to improve our Internet-based data acquisition and exchange capabilities and to develop a suite of general tools that could be applied to networking of remote field sites. For the second topic ECO sought to acquire and improve a general modeling framework that would be accessible to a wide range of ecologists, not just modeling specialists. Finally, ECO sought to link the two new capabilities as an integrated data acquisition and modeling framework running on a dedicated, internet connected server, with field data streaming in real-time to a general, process-based ecosystem model.

TECHNICAL PROGRESS AND RESULTS:

In the first two years ECO created specific tools such as the Research Platform software http://www.face.bnl.gov/data.htm, developed the ECO web site http://www.face.bnl.gov/eco.htm, revised and expanded the Windows Intuitive Model of Vegetation response to Atmospheric & Climate change (WIMOVAC) modeling framework and placed it onto our web pages http://www.face.bnl.gov/modelling/model.htm.

Work completed in FY2000 included:

- Installed and tested internet-based remote access and control capabilities.
- Developed SQL (Structured Query Language) database capability for ECO.
- Created a context-rich set of web-based information and data pages running on a BNL server http://www.face.bnl.gov.

- Created, maintained, and updated the ECO web site with links to field sites in order to obtain an early determination of the utility of such a community platform for data/science interchange.
- Verified the use of newly developed capabilities to acquire field data and to stream data in real-time to a general ecosystem model, WIMOVAC.

The discussions initiated as a consequence of the ECO LDRD have contributed to formulation of a request from OBER to BNL and ORNL for a "white paper" describing the need for Terrestrial Environmental Research Facility (TERF). It is anticipated that this will lead to support for planning such a facility and, eventually, to participation in development and research at a TERF facility.

SPECIFIC ACCOMPLISHMENTS:

The capabilities built by the ECO project contributed greatly to development of a successful proposal to DOE/OBER/TCP titled: "Eddy-Covariance Flux Tower and Tracer Technology Support for the University of Georgia Proposal: From Tower to Pixel: Integration of Patch-size NEE using Experimental and Modeling Footprint Analyses" (G. Hendrey and Russell Dietz). Funding for this new project is in the order of $700K over FY 2001-2003.

Humphries, S.; Behrens, W.; Lewin, K.; Nagy, J.; and Hendrey, G. 2000. FACE and Eco project Internet web pages: http://www.face.bnl.gov. Brookhaven National Laboratory.

Martin, M.J.; Farage, P.K.; Humphries, S.W.; and Long, S.P. 2000. Can the stomatal changes caused by acute ozone exposure be predicted by changes occurring in the mesophyll? A simplification for models of vegetation response to the global increase in tropospheric elevated ozone episodes. *Australian Journal of Plant Physiology*, 27.

Rogers, A.; Humphries, S.W. 2000. A mechanistic evaluation of concomitant photosynthetic acclimation and simulation at elevated CO_2. In press, *Global Change Biology*.

Martin, M.J.; Humphries, S.W.; and Long, S.P. A process-based model to predict the effects of climatic change on leaf isoprene emission rates. Accepted by *Ecological Modelling*.

Humphries, S.W.; Jones, M.B.; Long, S.P.; Morison, J.I.L. Development and testing a mechanistic model of papyrus (Cyperus papyrus L.) canopy carbon exchange using eddy covariance. Submitted to *Global Change Biology*.

LDRD FUNDING:

FY 1999	$346,900
FY 2000	$240,000

Parallel Algorithms For Accelerator Design

J. Glimm 99-10A
R. Samulyak

PURPOSE:

This project will explore novel simulation techniques which utilize parallel architectures and new algorithms for particle tracking and target design. Particle accelerators have defined the forefront of physics for most of the last century. Efforts to build the next generation of accelerators will involve unprecedented design challenges which can be met only by increased simulation and particle tracking. This includes machines currently under design, such as the Spallation Neutron Source (SNS), future machines such as the proposed muon collider, and the optimum use of current machines such as the Relativistic Heavy Ion Collider (RHIC).

APPROACH:

i) Accelerator Design

These problems represent a nontrivial challenge in that space charge and other multiparticle effects must be included. In order to study these effects the particle tracks as well as the interaction with the target material must be simulated. To do that the particle tracking codes have been extended so that a larger number of particles and multiparticle interactions can be included. This project will replace the fast fourier transform (FFT) solution of the Poisson equation with a matrix inversion scheme which is more suitable for particle tracking on a parallel computer.

ii) Muon Collider Target

The Muon Collider target will contain a series of mercury jet pulses of about 1 cm in radius and 30 cm in length. Each pulse will be shot at a velocity of 10-15 m/s into a 20 Tesla magnetic field at a small angle to the axis of the magnetic field. When the jet reaches the center of the magnet, it is hit with six 2 ns proton pulses during 6 ms; each proton pulse will deposit about 400 J/g of energy in the mercury. To handle the target a new stability study utilizing a linear stability analysis, a new representation of the equation of state of the target and a new algorithm to deal with the magneto-hydrodynamic effects associated with the intense confining magnetic fields were utilized. It is important to create an effective target able to generate the high-flux muon beam. The need to operate high atomic number material targets in particle accelerators that will withstand intense thermal shock has led to the exploration of free liquid jets as potential target candidates.

TECHNICAL PROGRESS AND RESULTS:

i) Accelerator Design:

Mathematically, one solves Maxwell equations to find fields and finally the angle kicks given the distribution of charges and currents. Current research has centered around the parallelization and expansion of two codes, ORBIT and SPINK. ORBIT is a particle tracking code that simulates the Spallation Neutron Source Accumulator Ring and SPINK is a tracking program used to study the dynamics of polarized protons in the AGS and RHIC. Both of these codes were originally serial and required extensive computer time for meaningful results. Both have been successfully parallelized using the Message Passing Interface (MPI) Expanding the capabilities of ORBIT is now the central effort. Implementation of the matrix inversion method to calculate force fields for the distribution of particles comprising the herd has been completed. This complements the original method of FFTs and has been found to increase performance. It also allows a more accurate treatment of the chamber walls to be included in the calculations.

ii) Muon Collider Target

Numerical simulations were performed using the computer code FronTier, developed to model the propagation of three-dimensional fluid jets. FronTier is based on front tracking, a numerical method for the solution of systems of conservation laws in which the evolution of discontinuities is determined through solutions of associated Riemann problems. The simulations show that the state of the mercury jet before its interaction with the first proton pulse is in good agreement with the linear stability analysis carried out as part of this project. A further result is that the surface instabilities of the mercury jet due to proton pulse energy deposition are not large enough to cause immediate break up into droplets. However, the observed surface instabilities will lead to jet break-up at a later time when the jet is leaving the magnetic field.

SPECIFIC ACCOMPLISHMENTS:

Galambos, J.; Cobb, J.; Holmes, J.A.; Olsen, D.K.; Luccio, A.U.; and D'Imperio, N.L., Parallel Tracking in Rings with Space Charge, EPAC2000 Conference Proceedings.

Luccio, A.U.; D'Imperio, N.L.; and Galambos, J., High Energy Accelerator Simulation and Parallel Computing, BANFF2000 Conference Proceedings.
Luccio, A.U.; and D'Imperio, N.L.; Tracking in Circular Accelerators with Parallel Computing ICAP2000 Conference Proceedings. (To be submitted to Physical Review Special Topics.)

Luccio, A.U. and D'Imperio, N.L. Tracking in accelerators with parallel computing. To be presented at the 6th International Accelerator Physics Conference, Darmstadt, Germany, Sept. 11-14, 2000.

Glimm, J.; Kirk, H.; Li, X.L.; Pinezich, J.; Samulyak, R.; and Simos, N. Simulation of 3D fluid jets with application to the Muon Collider target design. In M. Rahman and C.A. Brebbia, Editors, Advances in Fluid Mechanics, pp. 191-200. WIT Press, Southampton, Boston, 2000.

LDRD FUNDING:

FY 1999	$125,805
FY 2000	$170,000

Photonic Band Gaps In Nanostructured Materials

J. Glimm 99-10B
J. W. Davenport

PURPOSE:

Nanostructured materials offer great promise for the control of light (photons) in next generation optical devices. However, the propagation of photons in these structures is not completely understood at present. While studies of transverse electric (TE) modes have been successful we are aware of no comparable studies of transverse magnetic (TM) modes. The larger purpose of this project is the construction of a scalable parallel Maxwell equation code suitable for the simulation of finite optical devices.

APPROACH:

In order to extend the theory of these structures into the TM domain we have developed a parallelized, scalable Finite Difference Time Domain (FDTD) code to study photonic crystals. This code is capable of handling complex geometry, realistic initial and boundary conditions, finite size effects, dispersive and nonlinear media, and surface waves. Our primary focus is on the simulation of realistic experimental structures, such as waveguides, photonic band gaps and totally reflecting boundaries. In cooperation with J. Haus at University of Ohio, Dayton and Charles Bowden of Redstone Arsenal, we validate our code through a study of reflection, transmission and pulse propagation through photonic crystals. We propose to study such effects as group velocity, pulse dispersion and diffraction. Surface modes are relevant for example to antenna applications; wave guides and optical diodes are relevant to optical computing. We plan to combine our finite volume, time domain methods with adaptive gridding. The equations to be solved are Maxwell's equations, in the absence of charges, currents, or magnetic poles. The geometric complexity is introduced through the occurrence of discontinuities in the dielectric constant. Typically the interfaces on which the discontinuities occur will be separated by a fraction of a wavelength. (a quarter wavelength separation is typical for the production of a band gap.) These interfaces form a more or less repeated lattice pattern in two or three dimensions, thus giving rise to a photonic crystal, perhaps with irregularities, such as occurs with a wave guide embedded in the crystal. It is important to use adaptive gridding which conforms to the crystal geometry, including the surface of discontinuity of the dielectric. A regular grid will cover most of the computational domain, while geometric structures will be resolved adaptively using irregular grid elements.

TECHNICAL PROGRESS AND RESULTS:

Numerical results have been obtained for localized defect modes, excited by an oscillating dipole, in a two-dimensional photonic crystal with a triangular lattice consisting of an array of air cylinders in a dielectric medium (GaAs). They were calculated by using the finite-difference time-domain method on the Yee mesh. The results for the TE case were checked against experimental results and the numerical results from a different method. We have studied the spatial symmetry for different TM modes, obtained by changing the dipole excitation. Also, we have varied the defect radius and observed the changes in the resonant frequency. We discuss the localization as a function of frequency and studied the dependence of the eigenfrequncies on the size of the photonic lattice.

SPECIFIC ACCOMPLISHMENTS:

Stojic, N.; Glimm, J.; Deng, Y.; and Haus, J. W.; Transverse magnetic modes in two-dimensional triangular photonic crystals, to be submitted.

LDRD FUNDING:

FY 1999	$ 95,000
FY 2000	$140,000

Parallel Algorithms For Biomedical Image Processing

J. W. Davenport *99-10C*
A. Kaufman (SUNY/Stony Brook)
W. B. Lindquist (SUNY/Stony Brook)
K. Mueller (SUNY/Stony Brook)
Wei Zhu (SUNY/Stony Brook)
A. Dilmanian
M. Mcguigan

PURPOSE:

The purpose of this project is to develop advanced parallel and statistical based analysis and visualization techniques for comparing brain images, for automating the analysis of neurons damaged by ionizing radiation, and to aid in the development of treatment protocols in microbeam radiation therapy and in boron neutron capture therapy.

APPROACH:

i) BrainMiner

The main goal of this project is to discover and investigate correlational relationships of different regions of the brain. Evidence for these relationships is gathered by PET-imaging a number of human subjects, both under baseline conditions and under the influence of a drug. The correlations in the brain activity are calculated on the basis of predefined anatomical regions-of-interest (ROIs). The correlation coefficient is then employed to quantify similarity in response, for various regions during an experimental setting. The amount of statistical data can be enormous, and effective tools are essential if the brain researcher is to grasp and discover functional relationships quickly from the statistical data. BrainMiner is a visualization tool developed as part of this project which facilitates this task.

ii) Neuron Imaging

In order to assess the neurotoxicity of high-energy iron particles found in intergalactic cosmic rays, we used an *in vitro* model in which neuronal differentiation and neurite extension occur under controlled conditions. The model exploits chick embryo explants to study the effects of iron ions on neuritogenesis: a marker of functional neuronal integrity.

The imaging problem is to observe the growth of neurons regenerated from an explant and to quantify the extent of growth. The image analysis is a laborious task when done manually. Our algorithm has almost fully automated the image analysis, using as its basis the evaluation of a polar function of neurite density at each pixel.

iii) Radiation treatment protocols

There are two projects related to radiation therapies. The first involves 3D visualization of the Monte Carlo simulated dose distributions in tissues from the research program microbeam radiation therapy (MRT) that is being carried out at BNL. MRT is an experimental method of radiotherapy that uses parallel synchrotron-generated microplanar beams (microbeams), each typically 27 μm wide and up to several centimeters high with a 50-200 μm center-to-center beam-spacing. Half-power spectral energies of filtered white beams at the NSLS's X17B superconducting-wiggler beamline have been in the 50-80 keV range.

The second involves boron neutron capture therapy (BNCT) which is currently under investigation for the treatment of certain brain tumors. The protocol requires both an accurate image of the tumor and the development of a radiation dose schedule customized to individual patients. The effort is to improve on both aspects of this problem by utilizing a fast parallel algorithm along with a simulated annealing procedure to reduce significantly the time required to prepare for an individual patient and to provide a three-dimensional image of the tumor suitable for use by physicians.

TECHNICAL PROGRESS AND RESULTS:

i) BrainMiner

To test the software and develop its capabilities, PET fluoro-18-deoxyglucose (FDG) images were analyzed and displayed for two major drug addiction studies. Three major statistical measures were subsequently generated given the correlation matrix for each study: 1) Principal Component Analysis, 2) ROI cluster analysis and 3) Factor Analysis. The visualization interface displayed a 3D MRI volume coordinates which was sliced as three half planes of axial, coronal, and saggital views. The slices were drawn using 2D texture mapping. The correlation value was represented for each ROI as a color intensity in relation to a selected "root" ROI. In addition, all objects could be rotated together with the mouse (trackball interface) to provide a viewpoint from any direction.

ii) Neuron Imaging

To date, 580 images have been processed. Currently, we compare the amount of neurite growth with the size of the original explant. Future analyses will include counting the number of neurites as well as finding the length of the longest neurite.

iii) Radiation Treatment Protocols

We applied a grid of micro-beams to an egg-shaped $CaCO_3$ shell. We created a volumetric dataset from scan. Using volume rendering techniques one can clearly see the shape of the intensity variations of the microbeams. This method of visualization will be important in future applications of the technique.

The parallel simulated annealing approach has been implemented by defining a cost function associated with the radiation delivered to the tumor and target region and including constraints associated with the radiation delivered to the brain as a whole.

SPECIFIC ACCOMPLISHMENTS:

McGuigan, M. and Ma, R. BNCT Optimization By Parallel Simulated Annealing, Medical Physics, (submitted).

LDRD FUNDING:

FY 1999	$125,000
FY 2000	$180,000

Electron Diffraction Studies of Charge Ordering in Transition-Metal Oxides

Yimei Zhu 99-26
A.R. Moodenbaugh
J.M. Tranquada

PURPOSE:

Study charge ordering in strongly correlated electron systems, such as manganese perovskites with colossal magnetoresistance (CMR) and high temperature superconductors. The goal is to directly observe charge distribution, charge ordering and stripe phases, using quantitative electron diffraction, high resolution imaging, and nano-probe spectroscopy methods developed at BNL. The project results will have impact on the understanding of the high-temperature superconductivity mechanism.

APPROACH:

This project combines the analytical power of the EST transmission electron microscope (TEM) [1], along with x-ray and neutron scattering studies in the Physics Dept. [2]. Direct observation of dynamic charge and orbital ordering in superconducting oxides is very challenging. To achieve this goal, we pursue the study in two major phases. First, we study manganites, where the large atomic displacements associated with orbital-ordering assist the observation of charge ordering. Then we study the nickelate La_2NiO_{4+x}, which is structurally similar to first high Tc superconductor $La_{2-x}Ba_xCuO_4$. Controlled hole doping using oxygen content make the Ni-based system ideal to interpret the observed charge and orbital ordering. In addition, since the neutron scattering group in Physics has intensely studied La_2NiO_{4+x}, the sensitivity and accuracy of the TEM observations can be confidently compared with neutron data. Our approach utilizes advanced TEM methods, aided by computer simulation of electron diffraction and high-resolution images on a nanometer scale.

TECHNICAL PROGRESS AND RESULTS:

In early FY2000, the second year of the LDRD, we continued the study of charge ordering in $La_{0.33}Ca_{0.67}MnO_3$. Our focus was on the structural origin and evolution of twinning and the associated charge ordering during two phase transformations, from high-temperature primitive cubic (HTC) above 1073K, to room-temperature orthorhombic (RTO), and then, below 260K, to charge-ordered low-temperature orthorhombic (LTO). The existence of orientational domains associated with the reduction of the crystal symmetry due to the phase transformations was predicted by group-theory analysis and observed with quantitative transmission electron microscopy. In both RTO and LTO phases the orientation domain has six variants with fifteen possible domain boundaries which can be classified as two types of reflection twins, the 90° / m{100} and the 120° / m{110} twins. Two kinds of anti-phase domains and their domain interfaces, associated with the loss of translation symmetry, with lattice shifts of $a_{CO}/3$ and $a_{CO}/2$ also were predicted and observed for the LTO phase. Our work clarifies the widespread misunderstanding of twinning being equivalent to charge ordering in the system. We discovered that the twin domains characteristic of the RTO phase appear above the charge ordering temperature T_o and are not caused by charge ordering. However, the anti-phase domains, which can account for the observed small c_O-component of the incommensurate modulation at low temperature, are directly related to charge- and orbital-ordering in $La_{0.33}Ca_{0.67}MnO_3$. Figure 1 shows a high resolution image of the charge and orbital ordered structure in $La_{0.33}Ca_{0.67}MnO_3$ observed at 85K. The dots represent atomic columns with a spacing of ~0.54nm. The vertical dark and light band contrast represent the ordered stripes. A calculated image, top right, using the structural model to the left, agrees well with the experiment.

Oxygen-related charge order in La_2NiO_{4+x} was performed primarily at room temperature, with some at liquid nitrogen. A wide range of complicated superlattices, not reported by neutron and x-rays, was observed. We have identified six superlattices. Among them only the first was observed by neutron diffraction. This ordering appears associated with arrangement of oxygen interstitials. Atomic imaging has demonstrated beautiful twinning and ordered stripes. The discrepancy between TEM and neutron observations is not yet understood. A careful 3-dimensional analysis of the superlattice in real space as well as in reciprocal space both using electrons and neutron will be able to solve the mystery.

SPECIFIC ACCOMPLISHMENTS:

There were two invited talks, one presented at the 6th International Materials Research Society Meeting, Hong Kong, July 2000, and the other to be given at the 8th Conference on Frontiers of Electron Microscopy in Materials Science, Nov. 2000. The Fig.1 is being featured as a DOE highlight for scientific research endorsement. Reviewed publications: R. Wang, J. Gui, Y. Zhu, and A. R. Moodenbaugh, Phys. Rev. B **61** (2000) 11946; Journal of Natural Science, **46** 79-83 (2000), Wuhan University, China; submitted to Phys. Rev. B, "Crystallographic analysis of orientation variant and charge ordered domain in LaCaMnO."

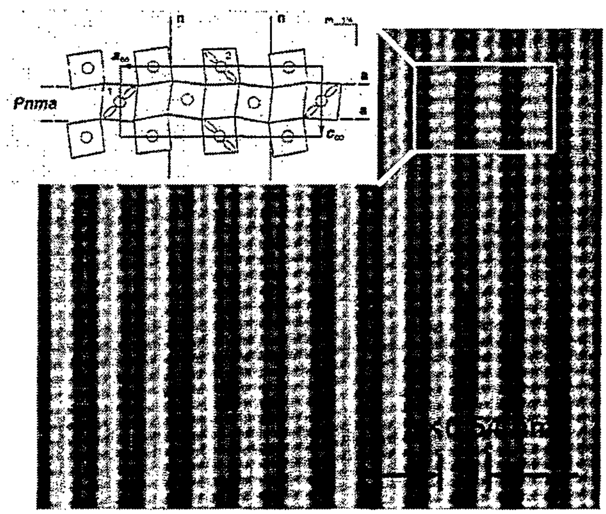


Figure 1. High resolution TEM image of the charge and orbital ordered structure in $La_{0.33}Ca_{0.67}MnO_3$ observed at 85K. The dots represent atomic columns with a spacing of ~0.54nm. The vertical dark and light band contrast represent the ordered stripes. A calculated image, top right, using the structural model to the left, agrees with the experiment.

REFERENCES:

[1] Yimei Zhu and J. Tafto, Phys. Rev. Lett. **76** (1996) 446.

[2] See, for example: J. M. Tranquada, et al., Nature (London) **375** (1995) 561.

LDRD FUNDING:

FY 1999	$86,793
FY 2000	$74,696

Evaluation of a Millimeter Quasi-Optical Source for Non-Destructive Detection & Analysis

M. Ruckman *99-28*

PURPOSE:

This LDRD program is to evaluate the use of a Russian-built millimeter quasi-optical source for non-destructive materials analysis. The Russian Back Wave Oscillator (BWO) technology was obtained through a separate IPP (Initiatives for Proliferation Prevention) project. The LDRD funding is to be used to test the BWO capabilities for the detection of unknown liquid or solid materials in packages.

APPROACH:

Sub-millimeter waves are ultra far-infrared or very high frequency microwave radiation. The BWO source used in this project resembles a traveling wave tube. An electron is directed through a slow wave structure that modulates the electron beam and establishes a periodic EM field. Fluctuations in the beam are amplified at a resonant frequency determined by the geometry of the slow wave structure, energy of the electron beam and strength of the magnetic field in which the BWO electron tube is placed. The BWO was engineered to produce a tunable sub-millimeter wave beam when the electron energy is ramped between several hundred to several thousand volts. The sub-millimeter wave signals are detected using a Golay cell. It has a dynamic range of 100,000 and can detect microwatt signals. Detection sensitivity can be increased using phase-locked detection. The continuous wave signal of the BWO was chopped. A Ni thin film attenuator is used to prevent the overloading of the Golay cell. The current set-up measures the optical transmission and phase of the transmitted beam. Physical parameters like the real and imaginary components of the dielectric constant can be computed using this information.

The initial experiments will get optical data for a few selected solids and liquids and the materials used in shipping packages. Materials such as wood, cardboard, leather and paper are chemically inhomogeneous, complex structurally, and “rough” when compared to samples normally studied by spectroscopists. Experimentation is necessary to determine how such complexity changes sub-millimeter transmission, beam coherence, or beam polarization. Additional experiments will test the ability of the spectrometer to detect solvents in plastic or glass bottles. Such work would provide data to determine whether a credible case can be made for the further development of a portable BWO-based technology for scanning.

TECHNICAL PROGRESS AND RESULTS:

During FY 2000, efforts focused on: (1) conducting transmittance and dielectric constant measurements of materials of interest to the program, and (2) testing the ability of the spectrometer to identify the chemical speciation of samples (spectroscopy of soft vibrational modes and high quantum number rotational transitions. The “Epsilon” spectrometer hardware was received in January 1999 and it was installed in Bldg. 703. A Russian scientist (Dr. Sergey Lebedev of GPI-RAS (General Physics Institute of the Russian Academy of Sciences, (Moscow, Russia)) came to Brookhaven in July 1999 to calibrate the spectrometer and instruct BNL personnel on its operation and maintenance. Dr. Lebedev is one of the specialists at GPI in the operation of this type of apparatus and wrote the GPI-RAS supplied software which performs data acquisition, data storage, and off-line analysis.

Work conducted in FY 1999 focussed on the acquisition of optical extinction data for several materials relevant to this research was obtained. In FY 2000 more materials were examined and measurements were extended to some liquid solvents. The solvents were used to evaluate the potential of GHz waves as unique spectral signatures for chemical identification. It was found that the rotational bands are severely broadened and the expected linewidth was at the limit of frequency stability and monochromicity of the BWO source beam (~ 100 MHz). Studies of optically thin methanol samples found that the current BWO system could detect 7 to 8 rotational transitions at 387 GHz. The investigator also used the quasi-optical microwave beams to detect changes in electrical cabling subjected to accelerated aging. No changes were detected.

SPECIFIC ACCOMPLISHMENTS:

A proposal entitled "Quasi-optical Microwave Imaging for Concealed Threat Agent Detection" was submitted to the Dept. of Energy, Office of Nuclear Non-Proliferation (NN-20) for consideration as a FY 2000 New Start.

LDRD FUNDING:

FY 1999	$ 84,768
FY 2000	$ 59,852

Microdistribution Studies of ^{10}B for Neutron Capture Therapy Using Transmission Electron Microscopy

Ruimei Ma 99-40
Yimei Zhu
Joseph S. Wall
James F. Hainfeld

PURPOSE:

In radiotherapy the dose that can be delivered to tumor cells is limited by the tolerance of the normal tissues within the radiation field. Boron neutron capture therapy (BNCT) is based on the neutron capture reaction ^{10}B $(n,\alpha)^{7}Li$. The combination of high linear energy transfer (LET) and a short range of the alpha (α) and ^{7}Li particles increases the statistical chances that ^{10}B-laden tumor cells will be rendered non-clonogenic ("killed") while contiguous, ^{10}B-poor tissues will be spared. The microdistribution of ^{10}B in both tumor and normal tissues is of critical importance to BNCT, since any tumor cells which do not contain at least 30ppm boron will not be killed and may give rise to subsequent tumors. The objective of this LDRD is to conduct a feasibility study on intracellular boron detection at the ppm level using two high-performance electron microscopes at BNL.

APPROACH:

Detection using secondary ion mass spectroscopy has given useful results previously, but a suitable instrument is not available at BNL. Since screening of many specimens is desirable and collaboration with a group at Cornell was very slow, a local alternative was proposed.

TECHNICAL PROGRESS AND RESULTS:

Progress in 1999 consisted of production and imaging of phantoms with known boron distributions. These were imaged by instruments in the Environmental Sciences and Biology Departments. Results were consistent with predictions of bulk detection limits, namely 0.2% boron in a carbon matrix with 10% accuracy and 1 µm spatial resolution. This was not sensitive enough for tissue studies if the boron were uniformly distributed. Two possibilities remained for use of the Electron Microscope (EM) approach. First, if the boron were in localized deposits the sensitivity might be adequate. Second, if the spatial resolution were high enough to restrict the number of carbon atoms in the beam to less than 1000, single boron atom detection might be possible. In that case the detection limit could be in the low ppm range.

Progress in 2000 focused on the question of whether the boron was concentrated in granules in the tissue. D. Slatkin prepared frozen mouse tissue with boron concentrations up to 600 ppm. Swiss mice were injected ip with unenriched ZnTCPH, a boron containing reagent. A solution of 3.5 mg/ml was injected 0.01 ml/gbw (gross body weight) 6 times over 2 days, then animals were sacrificed 4 days after the last injection. DCP (direct coupled plasma) absorption spectroscopy showed that the spleen then had accumulated 456 micrograms of boron per gram of tissue. The spleens were rapidly frozen and stored under liquid nitrogen.

J. Hainfeld took the frozen tissues to the National Institutes of Health (NIH) lab of Brian Andrews in Bethesda, MD, where they used a cryoultramicrotome to prepare 100 nm thick tissue slices suitable for EM. The sections were then freeze dried and examined in the electron microscope (Fig. 1).

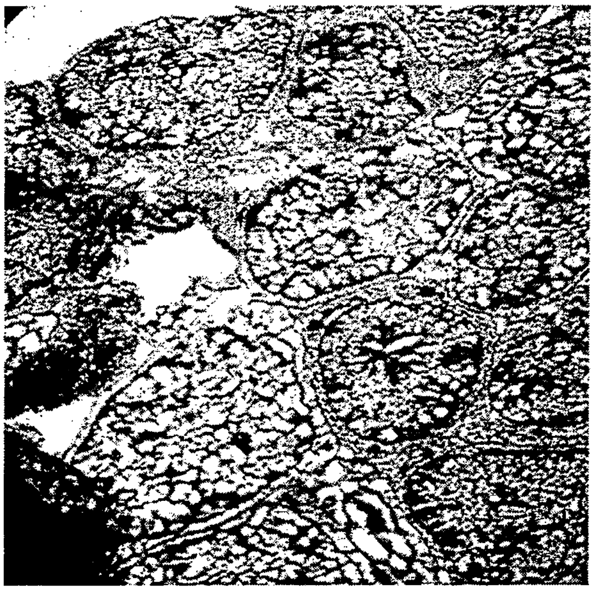


Fig. 1 Transmission electron micrograph of spleen of a mouse injected with a boron reagent, rapidly frozen, then cryosectioned and freeze dried. Several cells are visible, and the vacuolated appearance indicates some water crystal damage during freezing. Full width 25 microns.

Sections were also coated with a thin layer of carbon (for stabilization) and examined in the JEOL 3000F using the electron energy loss spectrometer (EELS). Because the sample was at or below the EELS detection limit, the boron maps obtained were noisy, and further work to either detect boron particulates or optimize STEM data collection from single boron atoms is necessary to improve detection.

Testing of single boron atom detection using STEM3 in Biology is continuing. This requires attainment of the ultimate in performance of all microscope components and this has been delayed by cutbacks in other DOE support. This goal still appears feasible but work has shifted to phosphorus detection, supported by other funds. However, instrument tune-up for phosphorus detection can easily be transferred to the boron work.

In parallel with the above research activities, an alternative boron mapping strategy was devised after searching the literature for available techniques matching the requirements for sensitivity and spatial resolution. A mass spectrometer microscope was proposed using a time of flight mass spectrometer and a small irradiation spot. With help from Bob Beuhler, Chemistry, and Ming Wu, ES&T, we set up a simple system with pulsed laser illumination. Results were limited by stray light reflected within the chamber, and it was clear that further development of the technique was beyond the scope of the available funding. The idea appears sound, however, and all the investigators involved are interested in pursuing it further in the future.

LDRD FUNDING:

FY 1999	$117,614
FY 2000	$ 58,867

Efficacy of Unidirectional Microbeam Radiation Therapy in Treating Malignant Tumors: Preclinical Studies in Rats and Mice

<u>*F.A. Dilmanian*</u> *99-41*
B. Ren
L. Peña
In collaboration with G.M. Morris, T. Bacarian, J. A. Coderre, E. M. Rosen, J. Tammam, and N. Zhong

PROJECT DESCRIPTION:

The goals of the present LDRD are: a) to evaluate in detail the tissue sparing effects of unidirectional MRT, and therapeutic efficacy using the rat 9LGS brain tumor model; and b) to establish the therapeutic efficacy of unidirectional MRT in several tumors other than 9LGS. The innovative aspects of MRT are that instead of a conventional unsegmented beam of x-rays (i.e., a broad beam) it uses parallel, microscopically thin, synchrotron-generated x-ray beams. MRT is single-fraction method, as opposed to conventional radiotherapy that commonly administers the dose in about 30 daily fractions in about 5 weeks. The high risk related to the MRT research program is that, like any other successful preclinical work, MRT research does not hold a firm promise for a successful future clinical stage. The challenge should be proper experimental design to address potential pitfalls in pre-clinical studies prior to potential clinical trials.

APPROACH:

Microbeam Radiation Therapy (MRT) is a novel experimental therapy method that uses arrays of parallel, microscopically thin slices of synchrotron x-rays. The microbeam arrays being used at the National Synchrotron Light Source (NSLS) have been 27- to 90-µm wide and up to several centimeters high, spaced 50- to 300-µm center-to-center, with a median beam energy of 50 to 120 keV.

TECHNICAL PROGRESS AND RESULTS:

The work completed in FY99 provided new experimental evidence on the two remarkable effects of single-fraction microbeam irradiation of animals, namely a) exceptional sparing of normal tissues, and b) tumor ablation or palliation at doses that caused no or little damage to the surrounding normal tissue.

The progress made in FY00 is summarized below. All the irradiations reported below were single-fraction and unidirectional. The doses are all surface doses; the doses for microbeams are in-slice ones. Except for the study with the rabbit eye and with the intracerebral 9LGS, all other studies used a 90-µm beam width and 300-µm beam spacing.

Studies with normal tissues

i. <u>Radiation tolerance of rat spinal cord:</u> Rats were irradiated on the cervical spinal cord with single-fraction microbeams and broad beams at 7-mm length of the irradiated cord. The end point was paralysis. The rats were observed for one year. Very high microbeam doses (600 Gy) were tolerated by the central nervous system without evidence of neurological impairment, whereas doses of 50 Gy and 75 Gy from broad beams resulted in paralysis.

ii. <u>Radiation tolerance of the normal rabbit eye</u> In this collaboration with Dr. S. Packer of North Shore Univ. Hospital, rabbits' eyes were irradiated with microbeams (27-µm width, 100-µm spacing) or broad beams. No damage to the retina was observed at 625 Gy microbeams a year after irradiations; the corresponding damage to the retina from 312 Gy broad-beam irradiation was substantial.

iii. Radiation tolerance of the normal rat skin
The end point was skin damage which was manifest as moist desquamation on the rat skin. The estimated ED50 (50% incidence) was 37.0 $\pm$ 0.1 Gy (SE) for broad beams and 836.8 $\pm$ 0.4 Gy for microbeams. The damage from microbeams was more superficial and transient. We conclude that normal rat skin tolerates microbeams at about 25-fold larger dose; this represents a 7-fold advantage when the dose is normalized to take into account the volume between the microbeams

Studies with animal tumor models:
i. Intracerebral 9LGS rat brain tumors
Unidirectional microbeams of 27-μm beam width and 50-, 75-, and 100-μm beam spacing were used. The end point was survival without morbidity. Histopathological analysis was used to assess the tumor stage/normal-tissue damage. Irradiations with 100-μm beam spacing at a dose of 400 Gy resulted in the most favorable therapeutic response, with about 67% survival at 180 days post-inoculation. There was no significant brain damage. This data points to a therapeutic index (i.e., the ratio of the dose which produces an unacceptable level of normal tissue toxicity to that required for tumor control) which is at least a factor of 2 higher, using the unidirectional MRT modality as compared with the broad beam modality.

ii. Subcutaneous murine mammary carcinoma EMT-6 Microbeam irradiations at 1672 Gy lead to 100% tumor ablation with normal tissue damage that involved hair loss and tissue shrinkage. Complete hair re-growth occurs at about two months after treatment. In contrast, 42 Gy broad beam irradiation of EMT-6 by other investigators lead to 80% tumor ablation with much larger level of normal tissue damage, where no hair re-growth was observed one year after treatment.

In summary, the proof of feasibility of MRT is that comparing single-fraction treatments in both MRT and broad-beam irradiations, MRT clearly has a larger therapeutic index in treating two difficult to treat animal tumor models, a glioma and a carcinoma. The first one was the intracerebral rat 9L gliosarcoma, and the second one was subcutaneous murine EMT-6 mammary carcinoma.

SPECIFIC ACCOMPLISHMENTS:

Publications: F.A. Dilmanian, G.M. Morris, G. Le Duc, et al. Response of avian embryonic brain to spatially segmented x-ray microbeams. Cellular and Molecular Biology (in press, 2000).

F.A. Dilmanian, G.M. Morris, G. Le Duc , et al. Microbeam radiation therapy: Therapeutic response of the rat 9L GS gliosarcoma. Journal of Neuro-Oncology (submitted).

Five abstracts were submitted to the 2000 Annual Report of the NSLS on Oct. 30, 2000.

Patent application: F.A. Dilmanian and G.M. Morris. Methods for Implementing Microbeam Radiation Therapy in Patient Treatment, Record of Invention submitted to BNL the Office of Technology Transfer, August 25, 2000.

Grant applications: A grant proposal was submitted to the Army's Breast Cancer Research Program in June 2000; review is expected in January 20001.

A grant proposal is being prepared for the OBER, U.S. DOE.

LDRD FUNDING:

FY 1999	\$119,571
FY 2000	\$149,204
FY 2001 (budgeted)	\$126,000

Toxin Bio-Information Resource

S. Swaminathan 99-45

PURPOSE:

Recent advances in molecular biology have made it possible to produce toxins which could be potentially used in wartime. These bioengineered pathogens could be produced in a large scale and sometimes introduced into a non-suspect protein. Chimeric Molecules form another form of threat wherein the virulent domain of a toxin is hidden in what is otherwise a non-pathogenic protein. The primary goal of this project is to create a database that will contain information about toxins, especially those that are potential biowarfare agents. The major objective is to develop a robust bio-informational resource that will collect, assimilate, synthesize, analyze and disseminate the basic molecular and structural information about potential biological warfare (BW) agents.

APPROACH:

The goal of the project is not only to assimilate all relevant information into a single database but also to provide query tools to search the database. This database will be created as a web-based system in which the required information could be retrieved by searching the database through key words, toxin name, name of the bacteria, etc. The basic approach will be to collect all relevant and available cellular, molecular, clinical, and structural information about toxins and related proteins through an extensive literature search and then to integrate them into one centralized database that could be used as an expert knowledge based system to learn about potential warfare agents.

TECHNICAL PROGRESS AND RESULTS:

The goal has been achieved to a large extent by designing a simple database. In the first step we have designed a schema to implement a highly curated Database System using Sybase which involves developing a schema consisting of different objects. Then a system was devised for identifying and maintaining important links between database objects and other information resources. The present database will be used for analyzing available information to determine the feasibility of developing potential warfare agents by enemy states. Our aim is to provide counter measures beforehand. Information and data are available in the database to identify and understand common motifs and structural patterns in these agents which would lead to developing counter measures such as detectors, drugs, and vaccines.

During the fiscal year 2000, we have developed a web-based database. In 1999, we had started this project by collecting data from selected toxins for the design of the database. In FY2000, this has been expanded to cover more potential toxins. Of these, 60 have already been entered in the database and others will be entered in due course. Based on the information and our analysis, we have developed a schema of the database which is being constantly revised and improved to make the database all encompassing and efficient. In the present system that we have developed, we have provided a web page based browser through which queries could be made. For example, a particular toxin could be searched by name, PDB entry number, Swissprot entry number etc. Information about each toxin is contained as one object with several sub-objects containing information about various aspects like molecular biology, structural biology, clinical information, etc., of the toxin. Dr. Ramon Miranda, an experienced biochemist, did an extensive literature search and gathered information about each toxin in the database and included annotations based on the information gathered. Lu Sun, an Information Systems graduate student at New York University, designed the database. We have now expanded our database to include toxins from other organisms also.

SPECIFIC ACCOMPLISHMENTS:

A web-site called Toxin Knowledge Base (TKB) has been developed (web address: http://avenger.bio.bnl.gov:8080/~tkb). This has been tested locally, and information about additional toxins is being constantly added. This web-site will soon be available for beta testing.

LDRD FUNDING:

FY 1999	$74,900
FY 2000	$75,760

Experimental and Theoretical Investigations of Transition Metal Oxides

J.P. Hill *99-46*
D. Gibbs

PURPOSE:

The purpose of this project is to push the development of new resonant x-ray scattering techniques in the study of transition metal oxides. These materials are interesting from both a fundamental and applied perspective. The new x-ray techniques shed light on the charge and orbital degrees of freedom which play a central role in determining the materials properties.

APPROACH:

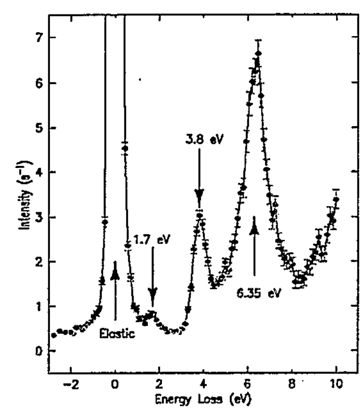
Work began in the manganite systems, to gain insight into both the systems themselves and the technique. The next goal was to extend the application of the technique beyond the manganites to other transition metal oxides.

Collaborators include Y. Murakmai (K.E.K.), V. Kiryukhin, and S.-W. Cheong (Rutgers U.), B. Keimer (MPI-Stuttgart), and Y. Tokura (U. Tokyo).

TECHNICAL PROGRESS AND RESULTS:

In FY 1999, we began investigating the $Pr_{1-x}Ca_xMnO_3$ system, studying the charge and orbital order using the new x-ray scattering techniques. This work revealed new insights into the ordering phenomena and produced high-resolution data for the theorists to use in calculating the various contributions to the scattering mechanism. Some preliminary work on some titanates was also performed.

In FY2000, we continued studying the $Pr_{1-x}Ca_xMnO_3$ system, focussing on the high-temperature behavior. By comparing $Pr_{0.7}Ca_{0.3}MnO_3$ with $La_{0.7}Ca_{0.3}MnO_3$, two systems with very different ground states, we assessed the role of the electron-phonon coupling in these systems. Remarkably, we found that at high temperatures these two systems exhibit similar correlations, which we interpreted in terms of bipolarons.



The work on $YTiO_3$ is currently being analyzed. We also began work on various nickelate and cuprate systems.

Finally, utilizing our new beamline at the Advanced Photon Source, completed in FY99, we began inelastic x-ray scattering experiments. The data illustrated above are for the cuprate ($CuGeO_3$). The peak at 1.7 eV arises from an orbital excitation. One of the goals of FY01 is to look for similar excitations in the manganites, where such excitations may form orbital waves ("orbitons") and exhibit dispersion.

SPECIFIC ACCOMPLISHMENTS:

Invited talks

1) Institute of Advanced Study Workshop, Santa Barbara, CA, November 1999.

2) ORNL Solid State Seminar, November 1999.
3) UIUC Solid State Seminar, December 1999.
4) MRS Fall meeting, Boston, MA, December 1999.
5) APS March Meeting Minneapolis, Minnesota, March 2000.
6) National High Magnetic Field Laboratory, Solid State Seminar, Tallahassee, Florida, April 2000.
7) International Jahn-Teller Symposium, Boston, Ma, August, 2000.
8) Workshop on Magnetic Scattering, Campinas, Brazil, August 2000.
9) International Conference on Magnetic Materials, Calcutta, India, October, 2000.
10) XRMS-2000, Berlin, Germany December, 2000
11) CMMP, Bristol, UK, December, 2000
12) Boston U. Solid State Seminar, December, 2000.
13) MRS Spring meeting, San Francisco, April, 2001

<u>Publications</u>

1) M. Von Zimmermann, J.P. Hill, D. Gibbs, M. Blume, D. Casa, B. Keimer, Y. Murakami, Y. Tomioka and Y. Tokura. Phys. Rev. Lett. **83**, 4872 (1999).
2) H. Nakao, K. Ohwada, N. Takesue, Y. Fujii, M. Isobe, Y. Ueda, M. von Zimmermann, J.P. Hill, D. Gibbs, J.C. Woicik, I. Koyama, and Y. Murakami. Phys. Rev. Lett. (submitted).
3) B. Keimer, D. Casa, A. Ivanov, J.W. Lynn, M. Von Zimmermann, Phys. Rev. Lett **85**, 3946 (2000).
4) J.P. Hill, D. Gibbs, Y. Taguchi, and Y. Tokura. Phys. Rev. Lett. (accepted).
5) I.A. Zaliznyak, J.P. Hill, J.M. Tranquada, R. Erwin, and Y. Moritomo. Phys. Rev. Lett. (accepted).
6) M. Von Zimmermann, J.P. Hill, *et al.* Informal Report (BNL 67265), Advanced Photon Source Activity Report.
7) M. Von Zimmermann, C.S. Nelson, J.P. Hill, D. Gibbs, M. Blume, *et al.* Phys. Rev. B (submitted).
8) V. Kiryukhin, B.G. Kim, V. Podzorov, S.-W. Cheong, T.Y. Koo, J.P. Hill, *et al.* Phys. Rev. B (submitted).
9) V. Kiryukhin, G.G. Kim, T. Katsufuji, J.P. Hill, and S.-W. Cheong. Phys. B (submitted).
10) Y. Murakami, J.P.Hill, D. Gibbs, M. Blume, *et al.* XVIIIth International Union of Crystallography Congress and General Assembly, Glasgow, Scotland, U.K., August 4-13, 1999.
11) J.P. Hill. In: X-ray and Inner-shell Processes, Ed. R.W. Dunford, et al., AIP, Conference Proceedings 506 (2000).
12) M. Von Zimmermann, J.P. Hill, D. Gibbs, M. Blume, *et al.* MRS Proceedings, Vol. 590, Application of Synchrotron Radiatio Techniques to Materials Science V, S.R. Stock, D.L. Perry, and S.M. Mini, Eds., ISBN: 1-55899-498-X.
13) M. Von Zimmermann, C.S. Nelson, J.P. Hill, D. Gibbs, M. Blume, D. Casa, B. Keimer, Y. Murakami, C.-C. Kao, C. Venkataraman, T. Gog, Y. Tomioka, and Y. Tokura. Workshop on Applications of Synchrotron Light to Magnetic Materials, Campinas, Brazil, August 14-16, 2000.

<u>Supported Researchers</u>

1 Post-doc (M. Von Zimmermann)
Travel to Advanced Photon Source.
Travel to selected meetings

Note: M. Von Zimmermann has obtained a permanent position at HASYLAB, Germany. In addition, in the past year two new post-docs have joined the effort (Christie Nelson and Young-June Kim).

LDRD FUNDING:

FY 1999	$84,400
FY 2000	$61,969
FY 2001 (budgeted)	$60,000

Pulsed Laser Deposition Facility

Peter D. Johnson 99-48
Barrett O. Wells
T. Venkatesan

PURPOSE:

Studies of correlated electron systems represent one of the forefront challenges in Condensed Matter physics at the present time. In particular, studies of the high T_c superconductors are the subject of a huge research activity. Photoemission represents one of the primary tools available for the study of these materials. However, one of the limitations of photoemission is that it requires well-defined surfaces. To date, therefore, the great majority of photoemission studies have concentrated on the cuprate $Bi_2Sr_2CaCu_2O_{8+\delta}$, which is cleavable. The Pulsed Laser Deposition (PLD) facility has been established with the express propose of extending these studies to other oxide materials that are not so easily cleavable. As an example growth of the $La_{2-x}Sr_xCuO_4$ type materials will be one of the primary objectives of the PLD program intially.

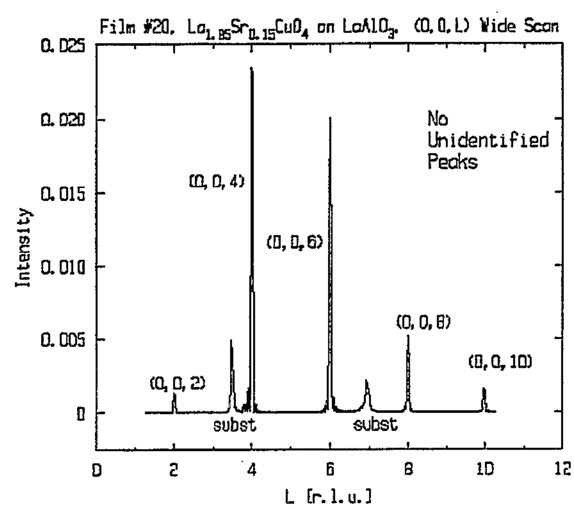
APPROACH:

A facility has been successfully established in the Physics Department under the leadership of Myron Strongin. Eventually it will be moved to the UV floor at the NSLS. The current plan is to commission the facility and grow samples in the Physics Department and then transfer them to various experimental end stations in some form of vacuum suitcase. When sufficient experience has been acquired, we will review the possibility of moving the facility to the NSLS.

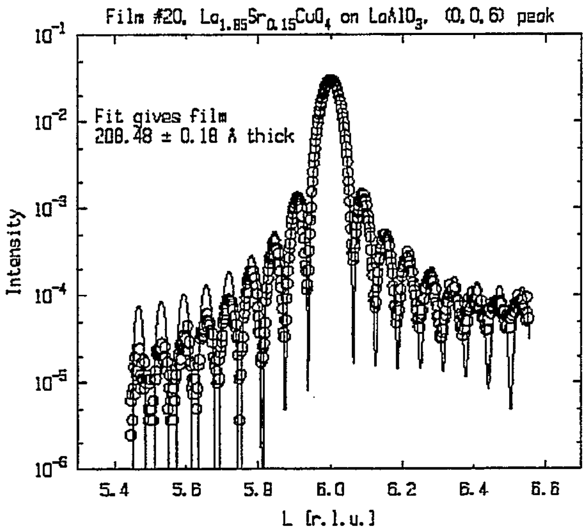
The project represents a collaboration between the University of Connecticut and the Physics Department, which was to establish an in-house materials growth capability based on the technique pulsed laser deposition (PLD). Another collaboration was established with the University of Maryland, where much of the U.S. effort in PLD is centered. The ultimate aim was and still is to be able to grow in-situ samples for use in different experiments at the National Synchrotron Light Source. The first objective was to grow samples that can be used in probes that are less sensitive to the surface condition including optical conductivity and x-ray scattering. However, a long-term concern is whether or not the texture of the surface will allow photoemission studies.

TECHNICAL PROGRESS AND RESULTS:

During FY 1999, a room in the Physics Department was equipped with all of the appropriate safety equipment and the laser installed and commissioned. During FY 2000, the first samples of $La_{1.85}Sr_{0.15}CuO_4$ were grown on $LaAlO_3$ substrates and studied with X-ray diffraction and resistivity measurements. The X-ray diffraction studies indicated that the films were of excellent crystalline quality as shown in figure 1.



Reflectivity studies indicated that the films had relatively smooth interfaces as shown in figure 2.



Resistivity measurements indicate that these films are superconducting with a transition temperature of 20K.

In FY 2001, good growth conditions will be established and initial measurements will be made at the NSLS using the technique infra-red spectroscopy.

SPECIFIC ACCOMPLISHMENTS:

The Condensed Matter Physics program has been successful in obtaining new money through the recent Complex Materials Initiative. A key component of the proposal was the stated intention of studying new materials fabricated using the technique of Pulsed Laser Deposition. The facility has also been included in the Laboratory's plans for Nanotechnology.

Work on $SrTiO_3$ has been submitted to Physics Rev. B for publication: - "Extreme strain effects on the structural phase transitions of SrTiO3 thin films," B.O. Wells, M. Von Zimmermann, S.M. Shapiro, Y. Zhu, A. Clark, and X.X. Xi.

LDRD FUNDING:

FY 1999	$122,300
FY 2000	$ 57,300

Ultrashort Electron Bunch Length Monitor

William S. Graves 99-50
Louis F. DiMauro
Richard Heese
Erik D. Johnson

PURPOSE:

This LDRD project supports the development of accelerator instrumentation designed to measure the length of sub-picosecond (ps) pulses of electrons.

Existing synchrotron light sources have pulse lengths of a few tens of ps. The next generation of light sources, including the DUVFEL at BNL, will produce intense pulses of light from ultrashort electron bunches less than 1 ps long. Such a beam presents new physics challenges and requires the development of a new class of instrumentation. The current state-of-the-art instrument for measuring short pulses is the commercially available streak camera, having a time resolution of 2 ps. The technical work described below is expected to improve this resolution by about one order of magnitude.

APPROACH:

To maximize the likelihood of success, several methods are being pursued in parallel.

The first method relies on the coherence properties of far infrared light emitted by the electrons in an undulator. In existing light sources with long electron pulses, the light emitted by each electron adds incoherently to that of all others in the bunch, so that the power produced is proportional to the number of electrons. However, if the bunch is short on the scale of a single wavelength of light, then the light from all electrons adds coherently, and the power emitted scales as the square of the number of electrons. This provides a very large enhancement of the power, as much as nine orders of magnitude. A short undulator, called COUR (Coherent Off-Axis Undulator Radiation), is installed in the DUVFEL accelerator to carry out this experiment. This work is the PhD thesis experiment of Charles Neuman from Duke University, and is being carried out in collaboration with Patrick O'Shea of the U. of Maryland.

The second approach also uses light from the COUR undulator. Rather than use the coherence properties of far infrared light, it uses the shot noise present in the visible part of the spectrum. Because there are a finite number of electrons in a pulse their single-shot spectrum is not smooth. Wavetrains from different electrons interfere in a characteristic pattern that depends on the length of the undulator and on the bunch length. For very short bunches this pattern can be resolved by a commercial spectrometer.

The third method is more risky, but also has the potential to provide the most detail about both the electron bunch and, eventually, about the short pulses of FEL radiation that will be generated by the DUVFEL. In this technique, the light from a fully coherent and well-characterized ultrashort pulse laser is mixed with undulator radiation from the electron beam in a nonlinear crystal to produce harmonic radiation. By measuring the spectrum of the harmonics as a function of optical delay between the two pulses, the complete amplitude and phase of the unknown undulator radiation pulse may be deduced. In the laser community this method has been used to measure the shortest light pulses (6 fs) to date. The extension that we are developing is to use two separate pulses rather than a single one. This is necessary because fairly high power is required to generate the harmonic radiation. We will employ one pulse from a high power, well-characterized laser, while the other is a low power undulator pulse of unknown structure. In the standard technique, a single relatively high power pulse is split and recombined.

TECHNICAL PROGRESS AND RESULTS:

In FY 1999, the COUR undulator that will be used in all of these experiments was rebuilt and the far IR optics designed and procurement started. A computer code to simulate the unusual properties of the coherent radiation was written and tested, and work on a paper describing the physics began. The visible/UV spectrometer was purchased.

In FY 2000, the COUR undulator was magnetically mapped and shimmed to meet precise specifications. Final assembly and installation into the accelerator beamline was then completed. The vacuum chamber and all in-vacuum diagnostics were built, tested, and installed in the beamline. The liquid He cooled bolometer used to measure the far IR spectrum was specified and purchased, and is currently being installed.

The DUVFEL accelerator also completed construction, and commissioning is currently underway. The study of the compressed pulse will occur in FY 2001 and will be funded by LDRD 98-23B.
Milestones of particular note are the completion and installation of the undulator, purchase and bench testing of all needed instrumentation, and commencement of bunch compression studies with the newly operational accelerator.

SPECIFIC ACCOMPLISHMENTS:

Peer reviewed publications:
Coherent off-axis undulator radiation from short electron bunches, C.P. Neuman,W.S. Graves, P. G. O'Shea, Phys. Rev. ST-AB (March 2000).

Other publications:
I am writing the section on fast instrumentation for the LCLS Conceptual Design Report.

A talk, *Coherent Off-Axis Undulator Radiation as a Bunch Length Diagnostic,* C.P. Neuman, was presented at the "LCLS Fast Instrumentation Workshop," held on March 3-4, 2000, with 26 attendees from eight institutions.

LDRD FUNDING:

FY 1999	$110,000
FY 2000	$ 65,000

High Gain FEL Amplifier

George Rakowsky 99-51A
William S. Graves
Erik D. Johnson

PURPOSE:

For High Gain Free Electron Lasers (FELs) to work as single pass devices at short wavelengths, very long wigglers will be required for the amplifier. These devices would (in principle) be most efficient if they can be built without gaps for diagnostics and trajectory correction magnets. The aim of this project is to demonstrate the approach experimentally.

APPROACH:

As a starting point we have obtained the 10-meter long NISUS wiggler (from a canceled Army program) to use for this proof-of-principle experiment. If the device can be measured and shimmed to the tolerances required for an FEL amplifier, it would demonstrate the viability of the long seamless wiggler design approach. Our measured data will be used as input to model an FEL amplifier, which will help establish realistic expectations for FEL performance.

TECHNICAL PROGRESS AND RESULTS:

In FY 1999, we contracted with STI Optronics of Bellevue, WA, the company which designed and built NISUS (Near Infra-red Scaleable Undulator System) for Boeing, to assist in the mapping of the magnetic field. STI's 3-meter long magnetic field mapper was modified to fit the tight confines of the NISUS geometry, and the full 10-meter device was measured in four overlapping scans along the magnetic axis. The positioning and alignment of the mapper to the undulator centerline was accomplished in collaboration with the NSLS Survey Group. The vertical (principal) field component was mapped using a Hall-effect magnetic field sensor; the horizontal component (nominally zero) was measured using a one-period long coil.

The initial magnetic field mapping was completed in early FY 2000 at a gap of 14.4 mm. The electron trajectory, computed from the second integral of the field along the axis, is shown in Figure 1.

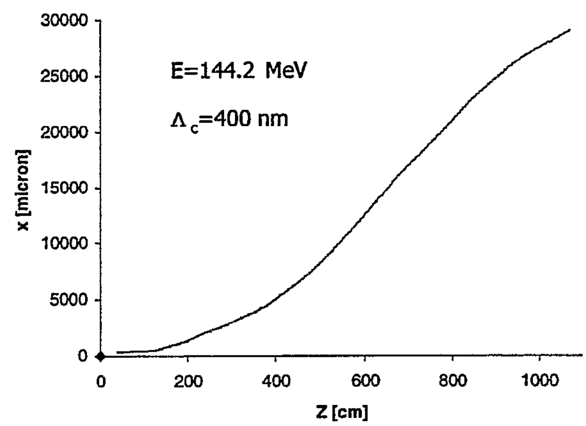


Figure 1. Calculated electron trajectory for NISUS undulator before shimming.

The cumulative effect of field errors results in a large walk-off from the magnetic axis, which would have even exceeded the aperture of the vacuum beampipe. In effect, the beam would have hit the wall.

For the shimming operation, the final gap was set to 20.6 mm, to achieve a peak undulator field of 0.31 Tesla for resonance at 400 nm with an electron beam energy of 144 MeV. To straighten the trajectory STI applied shaped steel shims of various thicknesses to appropriate undulator poles, according to a proprietary algorithm. The field was remapped, the trajectory recalculated, and the shimming process was iterated as necessary to reduce trajectory wander to less than a "wiggle amplitude" (approximately 25 μm) over each 3-meter scan length. The corrected trajectory, computed from the final four overlapping field scans, is shown in Figure 2.

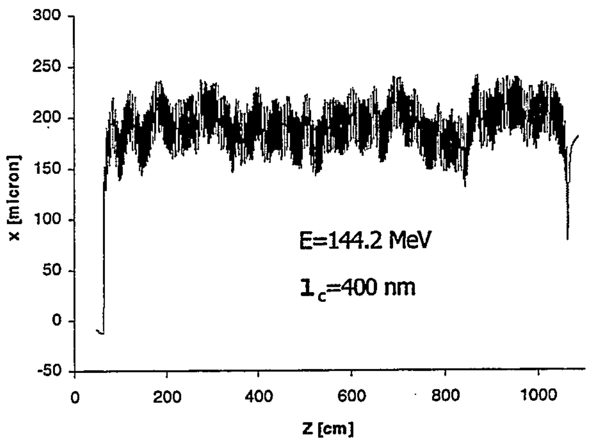


Figure 2. Calculated electron trajectory in NISUS undulator after shimming

After the trajectory was straightened over each 3m scan length, the "optical phase error" was computed. This parameter is closely correlated with FEL performance. Corrections were made in the local gaps to achieve a final rms phase error of only 4°, well within our requirements.

At each stage of field mapping, data was obtained not only along the geometric axis, but also off-axis at x = ±0.5 and ±1.0 mm, to determine transverse position sensitivity of the trajectory. Due to the use of canted poles (for two-plane beam focusing), off-axis fields differ from the on-axis field, resulting in systematic steering error equivalent to about 1.1 gauss/mm offset. This gives a measure of sensitivity to launch offset error.

Measurement of the small transverse, or "skew" field component in the presence of the large vertical field is difficult to do with a Hall probe due to non-linear cross-coupling within the Hall element. Instead, a scanning coil coupled to an integrating voltmeter was utilized to obtain this information. These measurements revealed a somewhat systematic skew field pattern with <1 gauss magnitude. Its cumulative effect (ignoring focusing) would be a vertical trajectory error of up to 2.3 mm. The skew field will be corrected with the 4-wire steering system built into the vacuum chamber using current settings derived from the measurements. Final steering corrections will be beam-based.

With the NISUS magnet shimmed and fully characterized, the vacuum chamber was assembled and installed. Still to be done in FY 2001 is making electrical connections to the 4-wire steering system, and completing the optical diagnostic system.

SPECIFIC ACCOMPLISHMENTS:

This work was presented at the FEL 2000 conference at Duke University August 13-18, 2000 Durham North Carolina 'Magnetic Measurements and tuning of the DUV-FEL undulator' S. Gottshalk, L. Campbell, STI Optronics Inc.

An invited report on the project was also presented at the Lasers and Short Wavelength Applications (LSWave) 2000 Meeting (a Satellite of the Synchrotron Radiation Instrumentation Meeting) at TU Berlin August 26 2000 'Overview of US Single Pass FEL Projects' E. D. Johnson

LDRD FUNDING:

FY 1999	$100,000
FY 2000	$100,000
FY 2001 (budgeted)	$184,000

Deep Ultra-Violet Free Electron Laser Optimization

Erik D. Johnson 99-51B
William S. Graves
Brian Sheehy
Li Hua Yu

PURPOSE:

Free Electron Lasers represent the frontier in accelerator based light sources. While there are many theoretical studies, there are relatively few experiments at short wavelength. None have yet monitored the FEL process as the photon and electron beams propagate though a continuous amplifier. This is especially important if tapering is to be used to provide energy extraction beyond FEL saturation. This project examines these issues experimentally and will provide data that can be used to qualify models for projecting the performance of future light sources.

APPROACH:

A critical element of the Deep Ultra-Violet Free Electron Laser (DUV-FEL) project is the optical amplifier. This requires a long magnetic undulator, electron beam diagnostics and controls, and an optical system to collect the light from the FEL and preserve its coherence as it is delivered to the experimental station.

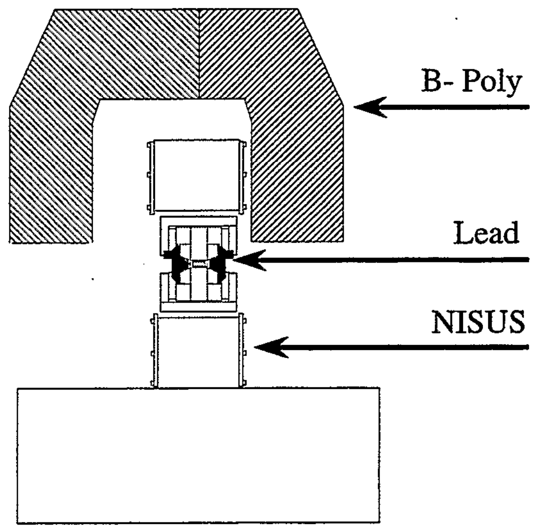
The US Army has transferred ownership of the NISUS undulator to BNL. This 10 meter long undulator is very flexible, and can be used to explore the way in which electron beam parameters influence FEL output. The vacuum system and diagnostics will be developed and assembled in the existing undulator. Light from the FEL will be relayed out to an optical table with a simple first surface mirror transport line. Initial experiments will be conducted in the visible due to the ready availability and high quality of optical diagnostics.

TECHNICAL PROGRESS AND RESULTS:

NISUS was built in 16 segments, each with its own four-wire steering section built into the vacuum chamber. Each section also has a port for a diagnostic probe to be inserted to measure the position and profile of the electron beam. We adapted designs from previous projects including the HGHG experiment and VISA to apply to the DUV-FEL and reported on the prototype design in last years progress report. We have made modest modifications to the design and have nearly completed the assembly of the full array of monitors (18) for the undulator.

These monitors represent significant electron loss points in the accelerator when they are inserted during operation. A shielding design study was undertaken to develop a method of providing adequate shielding without restricting access to the undulator or creating unacceptable loading its support table. Design of the shielding and verification of its performance were guided by simulations performed by Pavel Degtiarenko from TJNAF using codes developed for analysis of CEBAF.

The undulator magnet materials turn out to provide adequate x-ray shielding in the vertical direction, but additional shielding is required for x-rays that scatter to the sides. To minimize loading on the table, form fitting lead shielding was designed that is precast in small sections. The shielding allows for the required penetrations for diagnostics with the smallest possible opening.



Schematic of shielding components as viewed from the downstream end of the undulator.

To provide shielding for neutrons, it was found that borated polyethylene is required. As designed, the shielding is suspended over the undulator and can be moved away from the device for servicing through the use of an overhead rail system. Fabrication of the undulator shielding components is now underway.

Extensive thermal and vacuum cycling stability tests of the undulator vacuum system have shown a tendency of the chamber to creep by as much as 250 microns. The chamber carries the steering/corrector magnets with it when it moves. Motions of these magnets must be at or below the 30 micron level to assure an adequately straight trajectory of the electron beam through the wiggler. One of the activities planned for FY 2001 to address this problem is the development and installation of a laser alignment system that will allow measurement and correction of chamber position.

Installation of the shielding and transport of the electron beam to the wiggler are also planned in FY 2001. This will allow the first visible SASE experiments to be performed.

SPECIFIC ACCOMPLISHMENTS:

This work was presented at the SPIE meeting in San Jose in January 2000, 'The Deep Ultra-Violet Free Electron Laser (DUV-FEL) at Brookhaven National Laboratory' E.D. Johnson, I. Ben-Zvi, L.F. DiMauro, W.S. Graves, R.N. Heese, S. Krinsky, J.C. Sutherland, X. Wang, L.-H. Yu, in Biomedical Applications of Free-Electron Lasers, SPIE Vol. 3925 (2000) 26.

Presented a report at the Lasers and Short Wavelength Applications (LSWave) 2000 Meeting (a Satellite of the Synchrotron Radiation Instrumentation Meeting) at TU Berlin August 26 2000 'Overview of US Single Pass FEL Projects' E. D. Johnson.

LDRD FUNDING:

FY 1999	$400,000
FY 2000	$300,000
FY 2001 (budgeted)	$184,000

Development of High-Brightness Electron Sources

Ilan Ben-Zvi *99-53*

PURPOSE:

The objective of this work is to develop brighter electron beams from photoinjector electron sources. This is done through the development of innovative electron beam diagnostics and photoinjectors. This addresses the scientific issue of novel synchrotron light-sources by improving their brightness.

APPROACH:

The PI, in collaboration with other members of the BNL Accelerator Test Facility staff (in particular X.J. Wang, V. Yakimenko, M. Babzien and R. Malone, and research collaborators X.Y. Chang and S. Kashiwagi), undertook to combine the ATF's 'slice emittance' diagnostic and phase-space computer aided tomography to carry out these measurements and to develop an improved photoinjector.

TECHNICAL PROGRESS AND RESULTS:

In FY 1999, we made progress on beam transport analysis and control, RF phase control, Mathcad-based tomography software, electron-beam orbit correction, and photoinjector numerical simulations as described in detail in the 1999 report.

Progress in FY 2000:

1. Design Studies of a 120 Hz RF Gun for the LCLS: The starting point for the design is the BNL Gun IV, which demonstrated 50 Hz operation. Based on beam dynamics simulations we developed a new set of parameters for the photocathode RF gun injection system. We carried out a thermal analysis of the BNL Gun IV (Fig.1) and identified the possible hot spots. The cooling channel near the iris was increased and pushes close to the surface to improve the cooling capability.

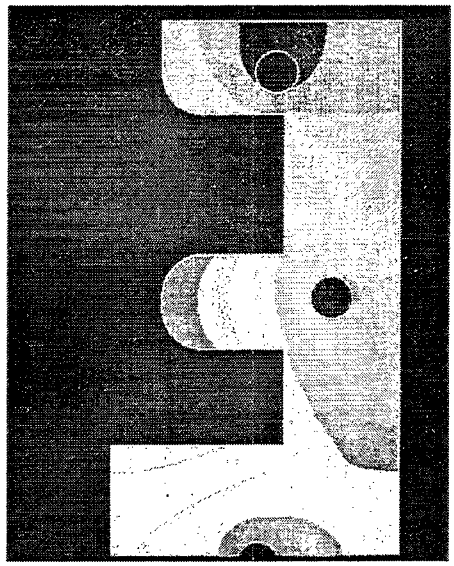


Fig. 1. BNL Gun IV thermal analysis for 1 kW CW power.

2. Photoelectron Beam Longitudinal Phase Space reconstruction using Tomography Technique: We measured the photoelectron beam longitudinal phase space as a function of the RF gun phase and charge using tomography (Fig. 2).

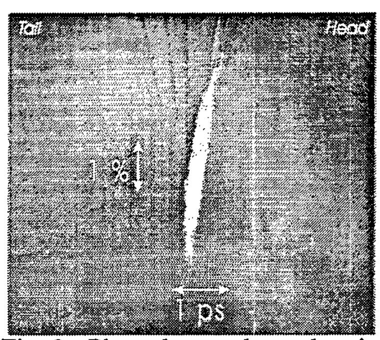


Fig. 2. Photoelectron beam longitudinal phase space reconstructed by tomography.

3. Photoelectron Beam Dynamics Studies: We have added features to the computer program PARMELA, to apply an arbitrary

laser longitudinal profile, which takes the Schottky effect into consideration, and perform slice emittance analysis (Fig.4).

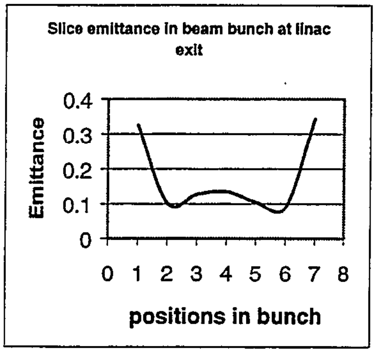


Fig. 4. Slice emittance (cm-mrad) as a function of position within the bunch.

The major results of this study are:

- Resolution of the disparity between theory and experiment on dependence of transverse emittance on RF phase,
- Identification of a laser distribution that produces a uniform electron beam distribution at small emission phases.
- Optimization of emittance as a function of the electron beam pulse shaping with a saturable absorber and electron beam shaping by an energy slit.

4. We performed a tomographic measurement of the transverse phase space distribution of three longitudinal slices of a beam.

Three 1.5 ps slices were selected out of a 5 ps well-optimized electron beam to analyze transverse phase space distribution. The normalized emittance of each slice was measured on the order of 1-1.2 μm. The emittance of the whole beam was measured at the level of 1.8-2 μm. From the phase space distributions (see Fig. 5) it is clear that the phase orientation of beam front and tail matches but not to the middle slice. That suggests that a longitudinally shaped laser can achieve further emittance improvement on the order of 30%. The fact that the emittance of each slice was on the order of 1 μm indicates that this level is limited not only by longitudinal dynamics but by other factors like non-uniformity of laser profile and cathode quantum efficiency. These issues should be addressed as well.

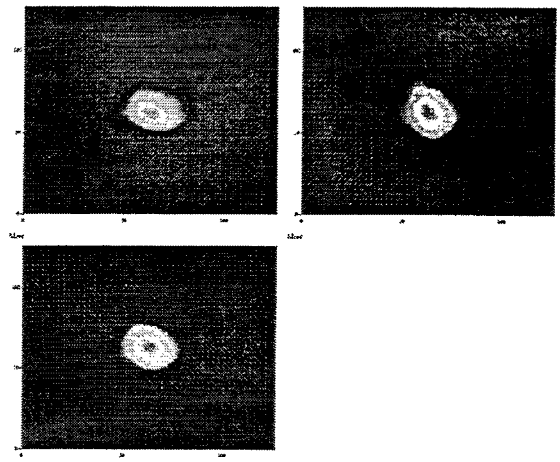


Fig. 5. Phase space density contours (false color) for three beam slices.

SPECIFIC ACCOMPLISHMENTS:

X.J. Wang, I. Ben-Zvi, R. Malone, V. Yakimenko, High-Resolution Beam Profile Monitor R&D At The BNL ATF, Conference: European Particle Accelerator Conference 2000, Vienna, Austria, June 2000.

S. Kashiwagi, M. Washio, X.J. Wang, I. Ben-Zvi, R. Malone, V. Yakimenko, Photo-Electron Beam Longitudinal Phase Space Tomography Studies At the ATF, Conference: 20th International Linac Conference, Monterey, CA, February 2000.

LDRD FUNDING:

FY 1999	$201,400
FY 2000	$199,807
FY 2001 (budgeted)	$100,000

Attosecond Pulse Generation in High Harmonics

Louis F. DiMauro 99-56
Brian Sheehy

PURPOSE:

The experimental realization of light pulses with attosecond time duration (10^{-18} seconds) would represent a new frontier in optical science and open new areas of research. The scientific interest encompasses atomic physics, femtosecond chemistry, and material science. The extreme bandwidth requirement of an attosecond light pulse renders conventional laser materials useless. One novel approach to this problem is the use of an extreme nonlinear process to generate a frequency comb of high harmonic radiation. In principle, the comb can extend from the ultraviolet to the soft x-rays, providing ample bandwidth for attosecond pulses. The key for achieving temporal compression depends upon the phase relationship between the electric fields of the harmonic comb. The objective of this proposal is to exploit the use of nonlinear processes for both the formation and measurement of attosecond pulses. BNL has prioritized 4th Generation Light Sources as part of the institutional plan and the DOE/BESAC committee has recognized attosecond pulse research as an important and integral part of this initiative.

APPROACH:

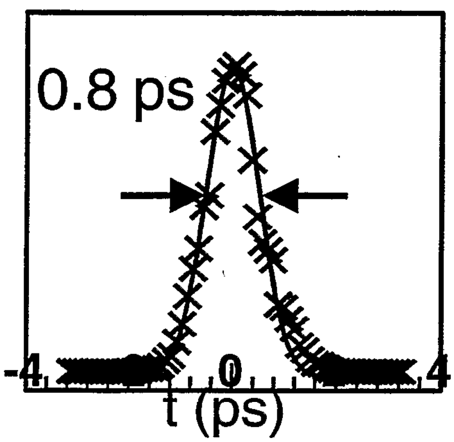
An intense mid-infrared (3-5 μm) atomic excitation is used to produce high harmonic radiation in a spectral (visible/near-UV) region accessible to common optical materials and well-established optical characterization methods, e.g. frequency-resolved optical gating (FROG). Theory suggests that the formation of attosecond pulses using high harmonic radiation is possible. Previous studies have established the correct physical scaling of the interaction of an intense laser with an alkali metal atom used in these experiments. Accurate measurements of the harmonic light can unequivocally establish whether an attosecond pulse can be formed and will serve as an important check in navigating the experimental difficulties involved in maintaining, measuring and using such pulses in real experiments. Attosecond pulses are extremely fragile, and our spectral measurements will tell whether the field and phase relationships necessary for the formation of the pulse exist, independent of the experimental complications that might cause the pulse to disperse before it reached the target.

These studies have been the work of Mr. Todd Clatterbuck (a SUNY Stony Brook physics graduate student) and a post-doctoral research associate, Dr. Claire Lynga.

TECHNICAL PROGRESS AND RESULTS:

In FY1999, we established the fundamental principles of our approach. High harmonics were produced from an alkali atom interacting with a long wavelength ($\lambda > 3$ μm) fundamental laser. The high harmonics produced in this manner emit in the visible/near-ultraviolet region of the electromagnetic spectrum. Thus, well-established techniques can be applied to measure the harmonics amplitude and phase.

In FY2000, we overcame many of the significant technical barriers for accomplishing the proposed science. We demonstrated the ability to generate a large enough number of harmonic photons to drive a nonlinear process and recorded the first autocorrelation temporal measurement of high harmonic radiation. *Autocorrelation and all the advanced optical metrology necessary to measure the relevant information for ultra-short pulses rely on a nonlinear interaction.* We designed and constructed an achromatic interferometer for recording an intensity autocorrelation (the same interferometer will be used in the FROG). The interferometer is all-reflective and uses off-axis parabolic mirrors as focusing elements. The entire optical system has excellent throughput with single photon sensitivity. An actual autocorrelation trace of the 5^{th} harmonic is displayed in the figure. This is the first time that such a measurement has been performed on high harmonic light.



In order to study the physics of attosecond pulses, our approach relies upon complete characterization of the high harmonic light and, equally as important, the fundamental pulse. Also in FY2000, we built a FROG apparatus capable of measuring the amplitude and phase of ultrashort pulses with wavelengths longer than 3 μm.

The objective in FY2001 is the application of the metrology, both autocorrelation and FROG, to high harmonic light. We will begin to study in detail the relationship between the fundamental and harmonic fields. Equally important is to gain an understanding of the entanglement of both the microscopic and macroscopic dipole phases.

We currently have solved the major technical issues associated with the measurement and studies in FY2001 will begin to shed light on the physics.

SPECIFIC ACCOMPLISHMENTS:

Two papers on the fundamental physics have been published in referred journals, these include Phys. Rev. Lett. **83**, 5270 (1999) and Phys. Rev. Lett. **84,** 2822 (2000).

L.F. DiMauro in FY2000 submitted a full proposal on attosecond science for a new DOE initiative entitled "Novel X-ray Sources." The proposal is a consortium of both national laboratory and university investigators. The status of this proposal with the DOE is pending a decision.

LDRD FUNDING:

FY 1999	$109,300
FY 2000	$ 77,988
FY 2001 (budgeted)	$ 75,000

Development of a 2-D Ion Imaging Detector for VUV-FEL Applications

M. White 99-57
R. Rao
R. J. Beuhler

PURPOSE:

We propose to develop an ion-imaging spectrometer for the study of surface reaction dynamics, which takes full advantage of the intensity and tunability of the proposed BNL DUV-FEL (Deep Ultraviolet Free Electron Laser). The spatial distribution of desorbed molecules from surfaces contains considerable information on the surface reaction and/or desorption dynamics, particularly with regard to the anisotropy of the molecule-surface interaction. Although ion-imaging has been used extensively in gas-phase studies, application to surfaces is not straightforward as the products are desorbed from a large source volume (crystal surface), and ionization is accomplished by a line source instead of a strongly focussed laser. Success of this project could help further the development of a scientific program for the DUV-FEL facility by providing a unique application of the FEL-generated VUV (Vacuum Ultraviolet) radiation.

APPROACH:

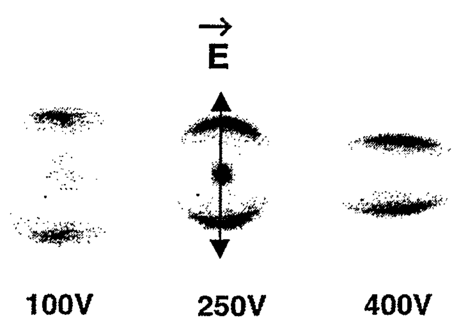
The main issues for design of the ion optics are (1) both the FEL and laser VUV beams are line sources over which ionization can take place and (2) the products originate from a distended source, *i.e.*, the metal substrate. We have adapted a new ion lens design, which has been recently demonstrated on gas-phase targets to dramatically improve the velocity focussing of ion-imaging systems. The 2-D spatial distribution of the ions is captured by a MCP-phosphor (Multi-Channel Plate-Phosphor) detector coupled with a video camera for full visualization. Image analysis software is also being developed to back-transform the raw images into velocity-resolved, spatial images of the desorbing products. The prototype 2-D imaging detector has been incorporated into an existing surface photochemistry apparatus equipped with a windowless VUV laser source for testing and optimization.

TECHNICAL PROGRESS AND RESULTS:

FY 1999: The SIMION 6.0 ion optics code was extensively used to evaluate lens designs for spatially imaging a distended ionization source. Ion trajectory simulations showed that the three-element, thin-lens design of Eppink and Parker (Rev. Sci. Instrum. 68, 3477 (1997)) had serious chromatic aberations for such large source geometries and additional elements would be required. Specifically, we found that a four-element system using thick ("tube") elements resulted in soft-focussing fields that could be tailored to provide imaging with source lengths as large as 2 cm. Simulations indicated excellent velocity focussing with lens voltages typical of time-of-flight spectrometers with moderate mass resolution ($\Delta m/m \leq 1\%$).

FY 2000: The lens design that meets both the space limitations of the spectrometer and the velocity focussing criteria was constructed and installed in an existing surface photochemistry apparatus for initial testing and evaluation. Significant modifications to the surface apparatus were required as the new imaging detector is considerably larger that the existing time-of-flight spectrometer. In addition, the software control for collecting images was installed and de-bugged and new image analysis software was evaluated.

Initial tests involved the use of gas-phase targets with well-defined fragment distributions to evaluate the lens design for velocity focussing using a line VUV ionization source. These tests showed that the lens element (V_3) added beyond the original Eppink and Parker design is crucial for velocity focussing and recompression of the image source. This is illustrated in the figure below for which coherent VUV radiation at 95 nm was used for excitation of H_2 gas. Dissociative ionization results in fast and slow H^+ ions that correspond to the outermost and central images, respectively. The ability to obtain high quality images such as these confirms the velocity focussing capabilities of our ion lens design for large source sizes. Current work is focussed on surface science applications where additional software analysis is necessary for reconstruction of the spatial images.



Series of three H^+ ion images for different values of the focussing voltage on the third element of the ion lens. The central image corresponds to complete velocity focussing. The ion source length is 1.8 cm. The direction of the polarization of the VUV radiation (95nm) is indicated (perpendicular to detector axis).

SPECIFIC ACCOMPLISHMENTS:

A summary of this work is being written as a paper to be submitted to the *Reviews of Scientific Instruments*. This work will also be the subject of an invited talk (MGW) to the Symposium on *Photon and Electron Induced Processes on Surfaces*, to be presented at the ACS Pacifichem International Congress, December 14, 2000, Honolulu, HI.

LDRD FUNDING:

FY 1998	$ 98,800
FY 2000	$ 78,291

Application of Quantitative MRI: Water Concentration and Blood-Brain-Barrier Permeability in Multiple Sclerosis

William D. Rooney 99-59
Patricia Coyle
Lauren Krupp
Joanna Smiroldo
Charles Springer, Jr.
Frank Telang

PROJECT DESCRIPTION:

The goal of this work is to develop and apply quantitative MRI techniques on BNL's 4 T scanner to better understand blood-brain barrier (BBB) function in health and disease. To achieve this goal we have studied healthy controls and multiple sclerosis (MS) subjects. MS is an autoimmune demyelinating disease of the brain and spinal cord that strikes an estimated 350,000 Americans. A well-known pathological hallmark of this disease is an abrupt and transient focal disruption of the BBB. It is unknown if subtle diffuse changes in BBB permeability occur in MS. This work is important for two reasons: 1) it will advance the technical capability of MRI to measure subtle vascular properties, and 2) it will contribute to fundamental understanding of perhaps the earliest disease pathology in MS amenable to imaging.

The specific objectives were to determine if: 1) brain water content is increased in MS white matter that appears normal on proton density MRI (so called "normal appearing white matter," NAWM) compared to control white matter, and 2) BBB permeability in MS NAWM is increased compared to healthy controls.

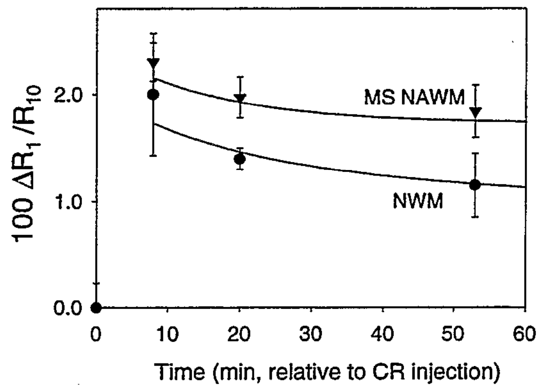
TECHNICAL PROGRESS AND RESULTS:

In FY 1999, we reported that brain water content was increased and that tissue concentration of a gadolinium (Gd) contrast reagent (CR) was increased at 20 minutes post injection in MS NAWM compared to control WM. We postulated that the increased tissue CR concentration was likely due to increased BBB permeability.

In FY 2000, quantitative MRI techniques were used to measure brain ^1H_2O T_1 values in controls and MS subjects before and after administration of a Gd CR. Since ^1H_2O T_1 is decreased by interaction of water with the paramagnetic CR, and in a concentration dependent manner, the tissue ^1H_2O T_1 values before and after Gd CR administration can be used to determine the concentration of CR in the brain. By following the temporal change in ^1H_2O T_1 after CR administration, modeling can provide parameter values for regional blood volume and blood to brain transfer rate constants for the CR.

Six healthy controls and four MS subjects were studied. Quantitative T_1 data was obtained before and at three times following a 30 s intravenous injection of 0.1 mmol/kg CR. At least eight regions-of-interest; 20 mm^2 or greater, were selected from the centrum semiovale and periventricular white matter.

The preliminary data are plotted as percent change in relative R_1 ($= T_1^{-1}$) in the figure. The solid symbols represent group average values with standard errors. At all time points the major contribution is from CR in the vascular space. The solid lines represent best fits obtained from a model function in which only two parameters were allowed to vary: 1) the regional blood volume, and, 2) the CR blood-brain transport rate constant.



For normal white matter (NWM) of healthy controls the parameters returned were consistent with those in the literature determined using radiotracers in the anesthetized rat. The modeling suggests that, on average, BBB permeability to CR was slightly increased in MS NAWM compared to control NWM. There is also a trend suggesting that RBV was increased. Our estimates are sensitive to the plasma concentration of CR and we have assumed an average temporal behavior of this quantity that is identical for both groups. High-field MRI instruments, such as the BNL 4 T scanner, provide superior CR detection sensitivity than standard clinical scanners which typically have magnetic field strengths of 1.5 T or less.

SUMMARY:

In MS NAWM compared to control white matter our data suggests the following: 1) water content is increased, 2) BBB is more permeable to CR, and 3) regional blood volume may be increased.

SPECIFIC ACCOMPLISHMENTS:

Collaborations

We continue two collaborations. The primary collaboration is with Drs. Patricia Coyle, Lauren Krupp, and Joanna Smiroldo of the Department of Neurology SUNY/Stony Brook. The objective of this collaboration is to use quantitative MR techniques to improve understanding of pathology of MS. The second collaboration is with Drs. Truman Brown (now at Columbia University), Michael Ochs, and Radka Stoyanova of the Fox Chase Cancer Center. The objective of this collaboration is to determine the utility of Principal Component Analysis and Bayseian techniques in improving the information content that can be extracted from brain water proton relaxographic imaging data sets.

Published Abstracts

1. Rooney, Telang, Krupp, Coyle, and Springer "Quantitative T_1 Mapping in Multiple Sclerosis Pre and Post Gd CR Administration" PISMRM 8:235 (2000).
2. Ochs, Stoyanova, Brown, Rooney, Li, Lee, and Springer. "Differences in T_1 Distributions Between Normal Volunteers and MS Patients Identified by Bayseian Decomposition Relaxographic Imaging" PISMRM 8:1183 (2000)

FOLLOW-ON FUNDING:

1. National Multiple Sclerosis Society (PI Rooney) "Quantitation of blood-brain barrier permeability in MS lesion development" 10/01/00-9/30/03 (Direct Costs $/year) $190,000
2. National Institutes of Health (PI Springer; Co-PI Rooney) "4 Tesla MRI Bolus CR Studies of Human BBB Permeability" 12/01/00-11/30/05 (Direct Costs $/year) $290,000
3. USB-BNL Pilot (PI Patricia Coyle, Co-PI Rooney)"Blood-Brain Barrier Permeability and the Menstrual Cycle" 11/01/00-10/31/01

LDRD FUNDING:

FY 1999	$74,443
FY 2000	$75,000

Study of Catalysts for SOx and NOx Decomposition Using Synchrotron Radiation

J.A. Rodriguez *99-62*
J.Z. Larese

PURPOSE:

There are two main goals in this project. The first one deals with the study and design of new catalysts for the removal or destruction of SO_x and NO_x compounds (i.e. DeSOx and DeNOx operations). The second one focuses on the development of synchrotron-based techniques for the characterization of these catalysts in-situ under realistic industrial conditions.

APPROACH:

Nowadays a major effort in environmental catalysis is focussed on reducing the content of sulfur and nitrogen oxides in the atmosphere. SO_2 and NO_2 are major air pollutants produced during the combustion of fuels in automotive engines, factories and power plants. There is a clear need to develop sorbents/catalysts with a high efficiency for DeSOx and DeNOx operations. Oxides can be quite useful in this respect.

In this project, the behavior of SO_x and NO_x species on oxides is investigated using a combination of several synchrotron-based techniques (photoemission, x-ray absorption near-edge spectroscopy, time-resolved x-ray diffraction) and theoretical methods (density-functional calculations). This allows a detailed study of fundamental problems for the design of a new generation of DeSOx and DeNOx catalysts.

TECHNICAL PROGRESS AND RESULTS:

In FY2000 we investigated the adsorption of SO_2 on ZnO(0001)-Zn. On the Zn terminated face of ZnO, sulfur dioxide was weakly bonded desorbing at temperatures below 200 K. Studies for the adsorption of SO_2 on MgO(100) and TiO_2(110) single crystals also revealed very weak interactions between the adsorbate and the oxide cations. The results of density-functional calculations indicated that in general the metal centers of an oxide interact poorly with the lowest-unoccupied molecular orbital (LUMO) of SO_2. This orbital is S-O antibonding, and the lack of strong interactions with the metal centers makes particularly difficult the dissociation of S-O bonds. To increase the DeSOx catalytic activity of an oxide one needs to create electronic states that interact well with the LUMO of SO_2. We have found that this can be accomplished in two different ways. One of them involves promotion with alkali atoms. This subject was partially explored in FY1999 for Cs/ZnO and K/ZnO. In FY2000, we tested this approach on a series of oxides (MgO, Al_2O_3, MoO_3, CuO, CeO_2) with satisfactory results. For oxides like Cr_2O_3, Fe_2O_3, TiO_2, and CeO_2, a decrease in the oxidation state of the metal centers favors interactions with the LUMO of SO_2 and dissociation of the molecule. Cr^{2+} and Fe^{2+} cations present in partially reduced Cr_2O_{3-x} and Fe_2O_{3-x} (respectively) display an extraordinary ability for cleaving S-O bonds. But we found that they easily transform into Cr^{3+} and Fe^{3+} (losing their catalytic activity) when present in pure chromium or iron oxides. In the final year of this LDRD (FY2001), we plan to prepare and test DeSOx catalysts in which Cr^{2+} and Fe^{2+} cations are trapped in a matrix of CaO, MgO or BaO. Recipes for the synthesis of these mixed-metal oxides are available and we can prepare the catalysts *in-house* or through collaborations with other research institutions and the industry.

Our studies have proved that x-ray near-edge spectroscopy (XANES) is an excellent technique for studying the chemistry of SO_2 on oxide surfaces. When compared to other techniques it allows an easy and precise identification of chemisorbed S, SO_2, SO_3 and SO_4 on the surface of oxide catalysts. At the present time, we are working in the development of instrumentation that will allow us to perform in-situ time-resolved XANES measurements at the NSLS.

In FY2000, we began to study DeNOx reactions on oxide surfaces. Important differences were observed on the reactivity of NO and NO_2 on MgO(100). Preliminary theoretical calculations and photoemission studies predict a high catalytic activity for mixed-metal oxides like $Fe_xMg_{1-x}O$, $Mn_xMg_{1-x}O$ and $Cr_xMg_{1-x}O$. In the final year of the LDRD, we plan to probe the catalytic activity of metal-doped MgO in DeNOx operations.

SPECIFIC ACCOMPLISHMENTS:

From the work done in FY2000, five articles have already been published or accepted for publication:

"Interaction of SO_2 with MgO(100) and Cu/MgO(100): Decomposition Reactions and the Formation of SO_3 and SO_4," J.A. Rodriguez, T. Jirsak, A. Freitag, J.Z. Larese, and A. Maiti, *J. Phys. Chem. B*, 104 (2000) 7439.

"Chemistry of NO_2 on CeO_2 and MgO: Experimental and Theoretical Studies on the Formation of NO_3," J.A. Rodriguez, T. Jirsak, S. Sambasivan, D. Fischer, and A. Maiti, *J. Chem. Phys.* 112 (2000) 9929.

"Experimental Investigations on the Interaction of SO_2 with MgO," A. Freitag, J.A. Rodriguez, and J.Z. Larese, *MRS Symposium Proceedings*, 590 (2000) 189.

"Chemistry of SO_2 and NO_2 on ZnO(0001)-Zn and ZnO Powders: Changes in Reactivity with Surface Structure and Composition," J.A. Rodriguez, T. Jirsak, S. Chaturvedi, and J. Dvorak, *J. Molec. Catal. A*, in press.

"Interaction of NO and NO_2 with MgO(100): Photoemission and Density-Functional Studies," J.A. Rodriguez, T. Jirsak, J.-Y. Kim, J.Z. Larese, and A. Maiti, *Chem. Phys. Lett.*, in press.

Our work has been very well received by the catalysis/surface-science community and the automobile industry. Two invited talks have already been given:

"Surface Science and Environmental Catalysis: Reactions of Desulfurization and Denitrogenation on Surfaces of Metals and Oxides," American Vacuum Society and North-American Catalysis Society: Michigan Chapters, Detroit, February 2000. (Sponsored by Ford and GM Company).

"Synchrotron-based Studies of the Chemistry of SO_2 on Metal and Oxide Surfaces," Second San Luis International Symposium on Surfaces, Interfaces and Catalysis, Mar del Plata, Argentina, April 2000.

And a third invited talk is scheduled for the near future:

"DeSOx and DeNOx Reactions on Oxide Surfaces" University of California at Berkeley, November of 2000.

LDRD FUNDING:

FY 1999	$122,000
FY 2000	$ 48,789
FY 2001 (budgeted)	$ 60,000

Exploration of The Object Oriented Approach To Reconstruction Algorithms

Howard Gordon 00-05A
Srini Rajagopalan
Bruce Gibbard
Torre Wenaus

PURPOSE:

BNL was recently selected by the DOE to serve as the principal computing center for U.S. ATLAS. It is vital that BNL's facility role be complemented by a strong core software program able to support the effective utilization of the center for U.S. based physics analysis. The purpose of this LDRD project is exploration of object-oriented approaches to reconstruction algorithms.

APPROACH:

We have pursued the development of analysis tools for high energy physics research using the most modern computing technology designed to handle the extreme scales in complexity and data volume reached by modern HEP experiments and particularly by the Large Hadron Collider (LHC) experiments. These new initiatives are building a pool of talent and experience at BNL that will position the Laboratory in the forefront of developing and deploying modern computing tools and support for High Energy Physics (HEP) experiments.

We have focused our efforts on specific areas of software development, chosen both for their exploratory reach into new technologies and for their impact on BNL capabilities if successful.

This focus area is the exploration of object-oriented approaches to reconstruction algorithms. We took as a specific example the Fortran-based reconstruction code for the ATLAS Liquid Argon Calorimeter (LAr). The objective was to explore the resources required to design and implement this code with a fully modern Object Oriented (OO) approach.

TECHNICAL PROGRESS AND RESULTS:

In the exploration of the OO approach to reconstruction algorithms, we have shown the approach to be successful in the timely and efficient development of reconstruction software meeting or exceeding the capability of the Fortran original. We implemented cell and clustering algorithms, corrections, and calibrations. Results in reconstructing test beam and simulated data have compared well to the Fortran codes developed over several years. We initiated an exploration of whether our codes can benefit from the OO event model developed by BNL and others for D0; this is being pursued with a prototype implementation in place.

SPECIFIC ACCOMPLISHMENTS:

Comparisons of the OO reconstruction developed in this project with previous Fortran codes met the quantitative requirements from ATLAS for reproducibility of simulation and test beam reconstruction results; our codes were subsequently accepted as the basis for ongoing development of OO LAr reconstruction in ATLAS. The success of this effort played a major role in the selection by ATLAS of one of us (S.R.) as LAr Reconstruction Coordinator for ATLAS.

(1) Proposal for an Object Oriented Liquid Argon Reconstruction
S. Rajagopalan
October 7, 1999, at Marseille, Liquid Argon Week
December 7, 1999, at CERN, Liquid Argon Week

(2) Progress with the Liquid Argon Reconstruction in the PASO Framework
S. Rajagopalan
February 15, 2000, ATLAS Software Week, CERN

(3) The migration of an Object Oriented Liquid Argon Reconstruction to the New ATLAS Framework (Athena)
S. Rajagopalan
April 17, 2000, ATLAS Architecture Workshop, CERN

(4) Tutorial on the Use of the new ATLAS Framework which included the Liquid Argon Reconstruction as one of the examples.
S. Rajagopalan
May 9, 2000, at Berkeley, CA
July 6, 2000, at CERN

(5) The Liquid Argon OO Reconstruction in the new ATLAS Framework
S. Rajagopalan
12 May 2000, ATLAS Software Workshop, Berkeley, CA

(6) Comparison of an Object Oriented Liquid Argon Reconstruction program with Fortran programming based software
H. Ma, M. Wielers
July 4, 2000, Liquid Argon Week, CERN

(7) Feedback to the ATLAS Architecture Review Committee on the integration of an Object Oriented Liquid Argon Reconstruction in the new ATLAS Framework.
S. Rajagopalan July 10, 2000 at CERN

(8) Status of the Object Oriented Liquid Argon Reconstruction Software
S. Rajagopalan August 31, 2000
ATLAS Software Week, CERN

(9) Proposal and Results of a Common Calorimeter Reconstruction Software Design
H. Ma, S. Rajagopalan, M. Wielers
23 October 2000, ATLAS Reconstruction Workshop, CERN

(10) Status of the Liquid Argon Reconstruction and electron identification
H. Ma, S. Rajagopalan, M. Wielers
28 November 2000
ATLAS Software Week, CERN

(11) Overview of the Calorimeter and electron-photon Reconstruction
H. Ma
December 6, 2000, ATLAS Liquid Argon Week

(12) A Hands-on Tutorial on the use of an Object Oriented Liquid Argon Reconstruction Software
H. Ma, S. Rajagopalan, M. Wielers
8 December, 2000 at CERN
A full day course attended by 15 people.

LDRD FUNDING:

FY 2000	$100,000

Assessment of Geant4 as a Model for the Atlas Liquid Argon Calorimeter Test Beam Data

Howard Gordon 00-05B
Srini Rajagopalan
Bruce Gibbard
Torre Wenaus

PURPOSE:

BNL was recently selected by the DOE to serve as the principal computing center for U.S. ATLAS. It is vital that BNL's facility role be complemented by a strong core software program able to support the effective utilization of the center for U.S. based physics analysis. The purpose of this LDRD project is the assessment of Geant4 as a model for the ATLAS Liquid Argon Calorimeter (Lar) test beam data.

APPROACH:

We have pursued the development of analysis tools for high energy physics research using the most modern computing technology designed to handle the extreme scales in complexity and data volume reached by modern HEP experiments and particularly by the Large Hadron Collider (LHC) experiments. These new initiatives are building a pool of talent and experience at BNL that will position the Laboratory in the forefront of developing and deploying modern computing tools and support for High Energy Physics (HEP) experiments.

We have focused our efforts on specific areas of software development, chosen both for their exploratory reach into new technologies and for their impact on BNL capabilities if successful.

This focus area is the assessment of Geant4 as a model for the ATLAS Liquid Argon Calorimeter (LAr) test beam data. Geant4 is a new software simulation package developed by a worldwide collaboration. It is based on the very successful Geant3 package which was developed at CERN in Geneva, Switzerland. It has been implemented in a fully Object-Oriented (OO) framework but has not been fully tested and validated as a physics tool.

TECHNICAL PROGRESS AND RESULTS:

In assessing Geant4 as a model for the LAr Calorimeter test beam data, we have compared results for energy and position resolution from Geant4 to actual ATLAS test beam data. After study we have identified discrepancies at the few percent level which we believe are attributable to the operation and physics modeling of Geant4. Resolution of these discrepancies is being pursued with the Geant4 collaboration.

SPECIFIC ACCOMPLISHMENTS:

Results of the OO reconstruction and Geant4 evaluation work have been presented in many meetings and workshops internally in ATLAS and externally in the community.

LDRD FUNDING:

FY 2000 $100,000

Probing Extreme QCD: Articulating the Physics Goals of an Electron-Relativistic Heavy Ion Collider (eRHIC) at BNL

R. Venugopalan 00-06
G. Garvey
T. Ludlam
L. McLerran
A. Deshpande

PURPOSE:

The purpose of this LDRD project is to explore the feasibility of building an electron-relativistic heavy ion collider here at BNL to study the hitherto unexplored regime of high parton densities in the theory of strong interactions--Quantum Chromo Dynamics (QCD). Similar studies have been performed previously exploring the electron nucleus collider option at the DESY Laboratory in Hamburg, Germany. The scope of the investigation is to perform a solid feasibility study that would be useful both to the Laboratory management and to the nuclear physics community at large in evaluating the scientific and technical merits of such a machine.

APPROACH:

Work has proceeded in several directions--through inviting the relevant technical and scientific experts for visits, reviewing scientific publications, conference talks of the principal and co-investigators, and the organization of workshops. These various avenues of communication and collaboration helped advertise the novel physics of an eA collider to the US nuclear physics community at large. They also helped highlight several open conceptual and technical issues. In particular, it was discussed how one could quantify the major theoretical uncertainties in the application of QCD to this regime. Technical issues regarding electron cooling, beam-Linac versus beam-beam, the number and design of interaction regions, were brought to the forefront. Long- and short-term visits of experts in these areas (particularly that of theory) were very useful in quantifying uncertainties in both conceptual and technical issues.

TECHNICAL PROGRESS AND RESULTS:

A year ago, eRHIC was a project that was in its infancy and completely unknown, outside a small circle, to the scientific community at BNL and outside. In little over a year, eRHIC is widely known both at BNL and in the wider community as a strong contender for a future DOE facility at BNL.

Three conferences/meetings were organized that were attended by many of the leading experts in the field: at BNL in December, at Yale in April, and again at BNL in the summer. It aided indirectly the writing of an accelerator design document by the RHIC accelerator group. A preliminary proposal for a detector design based on the ZEUS detector at DESY was made by W. Krasny at the Yale meeting. Significant progress was made by A. Sandacz at BNL in the summer of 2000 in quantifying the detector requirements for measuring semi-inclusive processes. Significant theoretical progress in understanding the high parton density regime of QCD was achieved by a (now former) post-doctoral fellow here, Dr. Yuri Kovchegov and Dr. Ian Balitsky of Jefferson Laboratory. They wrote down a very general equation describing properties of the high parton density matter--the predictions of this equation can be tested by eRHIC.

As a consequence of the rapid progress on several fronts (accelerator issues, detectors, and theory), we were joined by a large community of spin physicists primarily localized at MIT Bates Lab, the Indiana University Cyclotron Facility, and US members of the HERMES collaboration at DESY, Germany. Together with these physicists we are preparing a white paper for a future electron collider facility. This white paper will be presented at the Town Hall meeting at Jefferson Lab in December.

The next steps in the LDRD feasibility study is to make more quantitative several of the physics ideas associated with eRHIC. A post doctoral research associate, Dr. Jamal Jalilian-Marian from the University of Arizona is an expert on inclusive measurements of structure functions and has a keen interest as well in diffractive physics at eRHIC. He will help quantify some of the outstanding theoretical uncertainties in these areas. We also plan to invite key scientific visitors to BNL. Some of these are: a) Dr. Edmond Iancu from SACLAY in France, an expert on the physics of colored glass condensate that may be observed at eRHIC, b) Dr. Serbo from Novosibirsk, Russia, an expert on electron scattering and quark pair production, and c) Dr. A. Kaidalov, from Institute of Theoretical and Experimental Physics (ITEP), Russia, an expert on Pomerons in nuclei.

SPECIFIC ACCOMPLISHMENTS:

1) Established the eRHIC web page:
http://quark.phy.bnl.gov/~raju/eRHIC.html
This web site contains information about the various conferences organized, transparencies of talks, and various memos and reports. It also contains the report of the Accelerator Working Group on eRHIC.

2) Proceedings of the 2nd eRHIC workshop at Yale, April 6th-8th, 2000. BNL Formal Report No. BNL-52592
3) Proceedings of the BNL eRHIC summer workshop, June 26th-July 14th, 2000, to be published.
4) Several publications supported by LDRD funds:
a) A. Krasnitz and R. Venugopalan, Phys. Rev. Lett. {\bf 84}, 4309 (2000).
b) A. Krasnitz and R. Venugopalan, hep-ph/0007108, to appear in Phys. Rev. Lett.
c) R. Venugopalan, Pramana {\bf 55}, 73 (2000).
d) E. Iancu, A. Leonidov, and L. McLerran, submitted for publication, BNL-NT-00/24
e) A. Leonidov, hep-ph/0005010, submitted for publication, BNL-67422.
f) E. Levin et al., hep-ph/0007258, submitted for publication.
g) E. Levin et al., hep-ph/0007261, submitted for publication.

LDRD FUNDING:

FY 2000	$83,928
FY 2001	$85,000

Novel Techniques to Measure Aerosols

Stephen E. Schwartz *00-25*

PURPOSE:

The purpose of this project is to develop novel techniques to measure aerosol composition and physical properties rapidly and in real time, specifically (1) an aerosol sampler and analyzer, suitable for aircraft use, based on condensation of supersaturated water vapor, with capability for simultaneous measurement of positive and negative ionic constituents; and (2) a multiplexed tandem differential mobility analyzer based on a novel concept which permits the separation of particles into multiple packets of different sizes so that changes in relative humidity can be imposed and the growth observed simultaneously on the several size components. These measurement capabilities permit examination of the influence of humidity on the size of particles and relating to composition, permitting testing of understanding based on thermodynamic models. Rapid measurements permit many more samples to be obtained and economically analyzed leading to enhanced understanding of the spatial and temporal variability of these properties, information not presently achievable. These novel measurement capabilities will position BNL to be a lead participant in future DOE initiatives dealing with field measurements of aerosols and also to obtain funding from other sources for research on aerosol influences on climate and regional-scale air quality.

APPROACH:

Background. Atmospheric aerosols impair air quality affecting human health and welfare. Ability to develop effective and efficient strategies for control of aerosol loading and composition is currently constrained by measurement capabilities. Most previous work examining aerosol composition has been based on filter collection and subsequent analysis; sample amount requirements and analysis costs limit the time resolution of this approach to hours or days, and therefore important knowledge of temporal variation in composition is lost. Additionally, such filter-based approaches greatly constrain aircraft sampling by requiring long measurement periods for sample collection. Analysis and interpretation is further hindered because of long time delays before data become available.

Humidity analysis characterizes particle growth as a function of relative humidity, a key aerosol property, which gives insight into composition and which is directly pertinent to aerosol influences on climate, visibility impairment, and dynamics within human airways affecting deposition and ultimately health. Prior work has been limited by the requirement to sample one size at a time and the inherent slow rate at which the sample size can be scanned.

These considerations call for development of novel techniques for rapid real-time sampling of aerosols and for characterizing their physical properties and chemical composition.

Scope. This work consists of two parallel activities focusing on two new instrumental methods (1) particle-into-liquid sampler coupled to ion-chromatographic detectors for anion and cation species; and (2) multiplexed tandem differential mobility analyzer for simultaneous determination of humidity growth response of multiple particle sizes.

Key participants in this project were Yin-Nan Lee (particle-into-liquid sampler) and Fred Brechtel (multiplexed tandem differential mobility analyzer).

TECHNICAL PROGRESS AND RESULTS:

Particle-into-liquid sampler. A sampler and dual (anion and cation) analyzer for aircraft operation was constructed and tested. Initial field deployment was on the DOE Gulfstream-1 aircraft during the Texas 2000 Air Quality Study in Houston, August-September, 2000. An isokinetic inlet was coupled to an impactor to achieve a 2.5 µm particle size cut. Gaseous HNO_3, SO_2, and NH_3 were removed using two annular denuders in series before particles were activated for impaction and chemical analysis. Two compact ion chromatographs were used to analyze the cations Na^+, NH_4^+, K^+, and Ca^{2+} and the anions NO_3^- and SO_4^{2-} at a time resolution of 3 minutes. This system produced fast and quantitative airborne aerosol chemical data heretofore unobtainable. Data from 9/11/00 during a period with a southerly synoptic wind from the Gulf of Mexico, bringing in relatively clean air into the Houston region, are shown as an example below. Over the Gulf, the aerosol sulfate concentration was fairly low and exhibited a strong correlation with particle volume, indicating a rather constant aerosol sulfate content. During inland transects, this tight correlation no longer holds, suggesting a variable sulfate content. This observation is consistent with multiple sources of highly variable composition. Estimated sensitivity for sulfate is 0.1 µg m^{-3}.

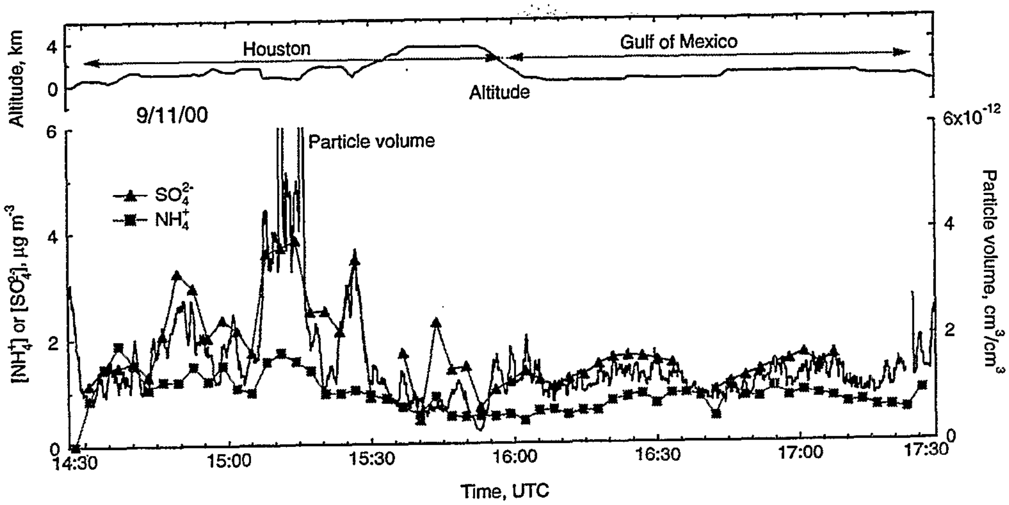
In FY 2001, a total carbon analyzer will be added in parallel to the ion chromatographs to determine the amount of organic aerosol.

Multiplexed Tandem Differential Mobility Analyzer. An instrument has been designed which will permit the sampling and separation of aerosols simultaneously into three different packets so that changes in relative humidity can be imposed on all three at once and the growth of each observed. The design is based on a conventional mobility analyzer but with three exit slits along the length of the central electrode instead of the usual single slit. The flow containing the particles of the three selected diameters will be subjected to a ramped relative humidity followed by particle sizing by time-of-flight analysis, permitting simultaneous determination of the humidity growth factors of the three selected particle sizes. Construction has begun.

In FY 2001, construction and design of the several system components will continue: particle condensational growth chamber, controlled particle humidifiers, multi-channel mobility analyzer, and time-of-flight detector. Initial testing will take place at BNL with field deployment in conjunction with other instruments in a field project later in the year. Experience with this initial instrument will allow final design features to be implemented and enable fabrication of a new instrument that will permit measurement of size-resolved water uptake for several relative humidities rapidly enough and with an instrument that is compact enough to be deployed on an airplane.

LDRD FUNDING:

FY 2000	$149,474
FY 2001	$242,000


Altitude, km
4
0
Houston
Gulf of Mexico
Altitude
9/11/00
Particle volume
SO$_4^{2-}$
NH$_4^+$
[NH$_4^+$] or [SO$_4^{2-}$], µg m^{-3}
6
4
2
0
6x10^{-12}
Particle volume, cm^3/cm^3
14:30
15:00
15:30
16:00
16:30
17:00
17:30
Time, UTC

Nanocomposites of Silicon Polymorphs and Related Semiconductor Systems

David O. Welch *00-27*

PURPOSE:

The goal of this project is to obtain a detailed understanding of the mechanisms of formation and the novel opto-electronic properties of nanocrystalline dispersions of metastable high-pressure polymorphic phases of Si and related semiconductor systems in normal diamond-cubic crystalline matrices, produced by shock-induced transformations resulting from high-velocity thermal-spray processing. This understanding will be achieved by high-resolution transmission electron microscopy and theoretical analysis, coupled with experimental measurements of opto-electronic properties. The technological promise is that this process is a potentially cheap and convenient way of synthesizing coatings for materials which exhibit novel functional behavior. The scientific issues which this work addresses concern factors which influence stress-induced phase transformations and factors which control retention of the metastable nanoscale phases. This requires an understanding of the stress-induced reaction pathways, the kinetics of subsequent relaxation reactions, and the role of retained internal stresses in the retention of metastable phases.

APPROACH:

This project is a collaboration between the Material and Chemical Sciences Division, Energy Sciences and Technology Department at Brookhaven National Laboratory and the National Science Foundation funded Materials Research Science and Engineering Center (MRSEC) for Thermal Spray Research at the State University of New York at Stony Brook. Recently the group at SUNY-SB demonstrated that thermal spray methods can be used to generate thick films of nanoscale composites of various polymorphic forms of Si. Si exhibits a number of high-pressure polymorphs, and upon depressurization, several metastable polymorphs, some metallic and some semiconducting, have been observed to result. Recently the group at Stony Brook has demonstrated that anisotropic shock synthesis, by means of thermal spray techniques, can be used to synthesize a fine dispersion (2-5 nm) of these metastable phases in a diamond-cubic matrix. The nature of the phases present, their size, and distribution depend on the characteristic velocity of the thermal spray process and on the orientation of the Si crystal substrate. This ability to produce nanoparticles of various metastable high-pressure phases of Si in a matrix of Si-I (the usual form) presents an excellent opportunity to study the mechanism of phase transformations in Si, as well as to study the properties of nanometer-size dispersions and their potential utility as opto-electronic materials. Furthermore the application of this method to other semiconductor systems (Ge, III-V compounds, etc.) is made in order to elucidate the role of such materials factors as ionicity and metallicity and to investigate their photo-conductive properties.

Joint discussions between BNL and SUNY-SB researchers led to the recognition that the capabilities at BNL for transmission electron microscopy (TEM) and theoretical analysis could greatly accelerate progress in understanding the mechanisms of formation and the physical properties of the nanocomposite system leading to the creation of this project. The work at BNL (LDRD-funded) consists of detailed TEM studies of the crystallographic and nanoscale structure of nanocomposites of group IV elements, as well as related III-V and II-VI compounds, which were synthesized by the Stony Brook group. This is accompanied by theoretical studies at BNL of possible mechanisms and kinetics of the nanocomposite formation mechanisms and of some of the physical properties of the nanocomposites. The primary personnel involved are Yimei Zhu (Scientist, BNL; electron microscopy), D.O. Welch (Sr. Scientist, BNL; theory), M. Schofield (Research Associate, BNL; electron micro-scopy), R. Goswami (Research Associate, joint BNL/SUNY-SB; electron microscopy and theory), S. Sampath (Prof., Materials Science and Engr., SUNY-SB; thermal spray processing), and R. Gambino (Prof. Materials Science and Engr., SUNY-SB; opto-electronic properties).

TECHNICAL PROGRESS AND RESULTS:

During FY 2000, a series of nanocomposite specimens of Si, Ge, C, BN, CdTe, and CdSe were synthesized using shock deformation induced by high-velocity thermal spray processing. By systematically varying the thermal spray parameters, various shock conditions were obtained and the resulting phases in the nanocomposites were correlated with shock-induced pressures, temperatures, and deviations. Detailed TEM studies were made of the nanoscale structure, including crystal-lography of the stress-induced metastable, nanoscale phases present in the resulting nanocomposites. The density and nature of crystal-lattice defects, such as dislocations and stacking faults, were also characterized by TEM. Variations of the nanoscale structure with crystallographic orientation of the single-crystal substrates upon which the high-velocity droplets impinged were observed and characterized. Theoretical analyses of the thermodynamics of transformations in Si were conducted, and the importance of the shear components of stress in determining the onset of phase transformation was established. A theoretical analysis was also made of nucleation kinetics and the importance of heterogeneous nucleation of phase transformation on shock-induced disloca-tions was revealed.

In FY 2001, a systematic study of the effects of ionicity of III-V and II-VI compounds and the tendency to metallization of the group IV elements on the nature and extent of the metastable phase formation and retention will be made and the theoretical analyses of thermodynamics and kinetics of shock-induced phase transformations will be extended to elements and compounds other than Si.

SPECIFIC ACCOMPLISHMENTS:

Two papers intended for submission to refereed journals are in preparation:

1) "Shock Synthesis of Nanocrystalline High Pressure Phases in Semiconductor Elements and Compounds," R. Goswami, H. Herman, S. Sampath, J. Parise, R. Gambino, Y. Zhu, and D.O. Welch.

2) "The Melting Transition in Nano-composites," R. Goswami and D.O. Welch.

A paper (F15.1) will also be presented at the 2000 Fall Meeting of the Materials Research Society, November 27-30, 2000, Boston: "Shock Synthesis of Nanocrystalline High-Pressure Phases in Si, Ge, and CdTe by High-Velocity Thermal Spray," J. Parise, R. Goswami, S. Sampath, R. Gambino, H. Herman, Y. Zhu, and D. Welch.

LDRD FUNDING:

FY 2000	$79,117
FY 2001 (budgeted)	$70,000

Preparation for Finalizing MATAC Installation

Lucian Wielopolski 00-28
Peter Thieberger

PURPOSE:

The technical objective of this work is to install a one-of-a-kind high intensity proton tandem accelerator, and bring it up to the design specification, i.e., beam current of 10 mA hitting a ^{13}C target. In this context, the exploratory nature of the work is that in this field there are no such machines with such high current. The prototype of this very same machine operated in a stable fashion at about 1.6 mA, and for a short time of operation reached 2.2 mA. The short-term technical implications include resolution of outstanding technical questions that undoubtedly will arise with regard to beam transport stability and target heating, and to demonstrate the feasibility to operate a DC machine at such high beam intensities. For that purpose alternative-engineering solutions will be sought. This LDRD is phase one in a multi-phase project that involves installing, testing, and developing four independent beam lines. The implications of a successful phase one are the development of four new long-term programs at BNL, one on each beam line; those coincide with the institutional and DOE developmental programs. Each of these programs requires a high intensity accelerator. In order of priorities, they are outlined below:

Nuclear Resonance: This is a unique analytical tool that requires a high intensity accelerator to produce specific gamma radiation through a (p,γ) reaction on a suitable target material. Subsequently, this gamma beam interacts resonantly with the nucleus of an element of interest, for example N, thus creating a unique signature of that element. This effect will be used in medical elemental tomography and for detection of explosives (detection of N). These two programs coincide and will add additional dimension to the Laboratory and DOE Imaging Science Initiative and strengthen the nonproliferation research.

Neutron Source: It has been demonstrated that using Li(p,n)Be and Be(d,n)B reactions produce intense neutron sources, about 10^9 n/cm^2/sec, with adjustable energy are possible. Closure of the Brookhaven Medical Research Reactor (BMRR) stripped BNL of the last available neutron source on site. Undeniably this will impede the progress in developing a binary approach to cancer treatment studies, which are carried on presently at the BMRR. This project coincides with the DOE initiative to develop cell-target ablation therapy using *in vivo* radiation techniques.

Analytical Tool: The high intensity charged particle accelerator is extremely suitable as an analytical tool for elemental surface and bulk analysis, not available at present at BNL. The variety of methods available, e.g., Proton Induced X-ray Emission, Proton Induced Gamma Emission, Rutherford Back-Scattering, Micro-beam, etc., provide a powerful addition in the armament of analytical tools available at BNL. The capabilities of micro- and interface- analysis with monolayer special resolution will support developments in Bioengineering and Nano-technology.

Ion Implantation: This high intensity accelerator is very suitable for high-energy (~ 2 MeV) ion implantation. At present, extensive work is being devoted toward developing accelerators for that purpose.

APPROACH:

The motivation for this project, as was stated above, required a special high intensity accelerator at about 2 MeV. The Federal Aviation Administration was developing this accelerator for the purpose of detection of explosives. Before it was finalized BNL assumed ownership of it and is at the stage of finalizing the installation. A team of experts with experience in electrostatic accelerators is available to assist in reaching the final design parameters. We are also in consultation with engineers from TRIUMF, in Canada, who were responsible for developing the High Voltage Power Supply for this accelerator. During assembly of the facility, there will be a learning curve to reach the final specifications. Problems will be resolved as they arise.

Collaborators from the accelerator department include: J. Alessi, D. Raparia, T. Russo, V. Zajic and others, as needed. In addition S. Malnuczyk, and J. Sradniewski from Advanced Energy Systems provide consultation as needed.

TECHNICAL PROGRESS AND RESULTS:

In FY 2000, significant progress was made in preparing and activating the proton injector. There was a delay of three months to address all of the ES&H concerns prior to activating the injector. Subsequently, a beam scanner was installed and commissioned. The BNL staff introduced several improvements in the scanner software, related to the data structure and display of the scans. The know-how to operate the scanner was also transferred from Advanced Energy Systems Inc. to BNL. Beam scans for different injector operating parameters were performed. Results are scans that will be evaluated in the next stage. The project will continue with the installation of the accelerator. It is anticipated that during fiscal year 2001 installation and operation of the tandem accelerator will be accomplished. Additional support for this project is sought from NIH and DOE, a grant has been submitted to NIH.

SPECIFIC ACCOMPLISHMENTS:

Publication and grant submissions to use the tandem accelerator have been submitted.

Publications:

1. Wielopolski ,L.; Ludewig, H.;Powell, J.R.; Raparia, D.; Alessi, J.G.; Alburger, D.E.; Zucker, M.S.; and Lowenstein, D.I.; Experimental and Theoretical Evaluation of Accelerator Based Epithermal Neutron Yields for BNCT. In Application of Accelerators in Research and Industry, Eds. J.I. Duggan and I.L. Morgan, (1999) 1033-1036.

2. Wielopolski, L.; Vartsky, D.; Pierson, R.; Goldberg, M.; Heymsfield, S.; Yasumura, S.; Melnychuk, S.; and Sredniawski, J.; Gamma Resonance Absorption New Approach in Human Composition Studies. In Vivo Body Composition Studies, Eds. S. Yasumura, J. Wang, R. N. Pierson Jr., Annals of the New York Academy of Sciences, 904 (2000) 229-235.

Presentations:

1. Fifth International Symposium on In Vivo Body Composition Studies, "Gamma Resonance Absorption: New Approach in Human BC Studies," Brookhaven National Laboratory, Upton NY, October 7-9, 1999.
2. Fifth International Symposium on In Vivo Body Composition Studies, "Operating Characteristics of a High Current Tandem Accelerator for Nitrogen Imaging in Human Bodys," (Co-author) Brookhaven National Laboratory, Upton NY, October 7-9, 1999.
3. DOE/OBER Medical Sciences Division Presentation. "MATAC: Medical Applications Tandem Accelerator," Germantown Maryland, January 15th, 2000.
4. NIH/NCI Biomedical Imaging Program, "Multiple Applications of a Tandem Accelerator in Bioengineering, Basic, and Clinical Research," Bethesda Maryland, May 1st, 2000.

Grant Applications:

1. DOE-OBER-FWP, Low Energy High Intensity Proton Tandem Accelerator for In Vivo Elemental Imaging & Neutron Production, 2000.
2. DOE-OS Notice 00-29, Pre-Proposal, Design and Construction of an Accelerator Based Neutron Producing Target/Filter for Medical Applications, 2000.
3. NIH-NIDDK, In Vivo Quantitative N Analysis and Imaging Using GNRA, 2000.
4. DOE-NN1-NN20 Detection and Imaging of N with 9.17 MeV Resonant Gamma Rays, 2000
5. CTTSO-TSWG High Explosive Detection and Imaging With Resonant Gamma Rays, 2000

LDRD FUNDING:

FY 2000	$ 58,480

Fig. 1 Location of the tandem accelerator in Building 945.

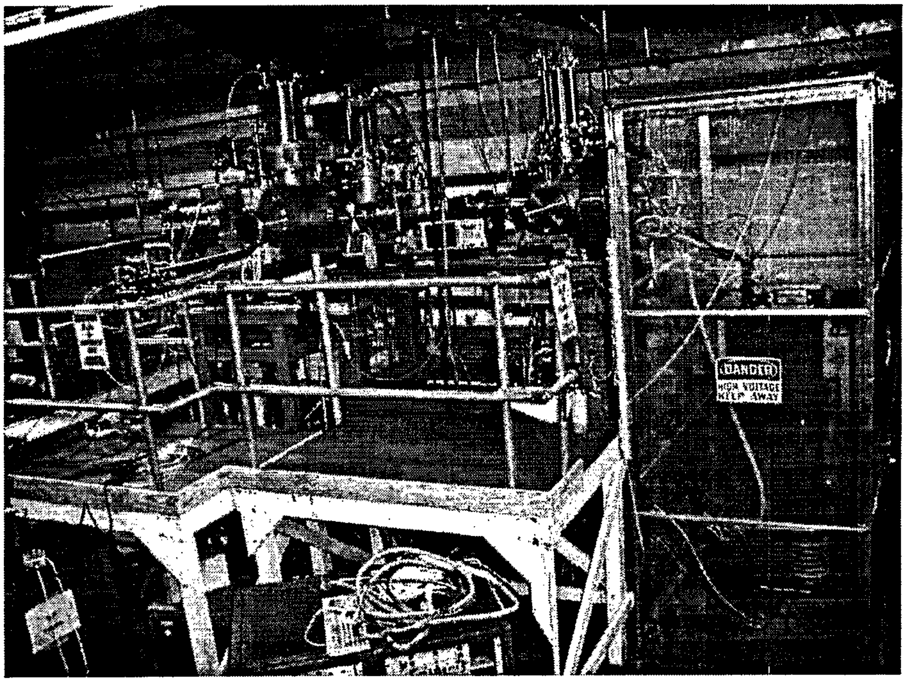


Fig. 2 Injector and the beam scanner installation in building 945.

Microvascular Endothelial Cells as Targets for Ionizing Radiation

Louis A. Peña, Ph.D. *00-32*

PURPOSE:

This LDRD supports the establishment of *in vitro* models of brain microvascular endothelial cells (EC) for radiobiology studies. A variation of the basic methodology permits the establishment of *in vitro* models of Blood Brain Barrier (BBB). These models will allow us to initiate a new program of basic and applied research of relevance to Radiobiology and Radiation Oncology, using modern cell- and molecular biology techniques. These model systems are not only important for our own project but will also promote future collaborations with other investigators/projects at BNL (e.g., neuro-imaging drug development [S.J. Gatley], neuro-imaging and the BBB [W. Rooney], microbeam radiation therapy [F.A. Dilmanian], radiation-induced cell death of CNS glial cells [L.A. Peña]).

APPROACH:

A significant portion of radiation injury arising from the therapeutic use of ionizing radiation is attributable damage to blood vessels. Microvascular endothelial cells are the cells of which capillaries are composed, and are the cells which line the inner lumen of large blood vessels (e.g., arteries and veins). The ability to modulate the radiation tolerance of ECs would be of significant therapeutic utility. Basic research into mechanisms of cellular responses to radiation is therefore of significant utility. Much of what is known in this area was done by Radiation Oncology researchers before the advent of modern molecular biology. To apply modern tools to this general problem, reliable *in vitro* models (cell culture) are required. The specific study of blood vessels and angiogenesis (Vascular Biology) is a specialized field in its own, and we need to draw experience from this area in order to apply it to the specific radiobiological questions.

This phase of the LDRD work is essentially a testing phase. In the upcoming period we will devote more effort to experimental work to advance the science. We obtain primary bovine or human endothelial cells from a commercial supplier (Clonetics-BioWhittaker). These cells are grown in tissue culture-treated plastic dishes without additional attachment factors. These dishes consist of standard laboratory flasks (25 or 75 cm^2) and petris (100 mm) as well as specialized chamber slides (Nalge/Nunc). The latter are used for microbeam studies at the NSLS in collaborations with Avraham Dilmanian (BNL Medical Dept.), and separately with Itzhak Orion (Weizmann Institute) & Zhong Zhong (BNL, NSLS).

We are testing basic growth kinetics in combination with Flow Cytometry analysis of the cell cycle to reproducibly obtain either quiescent or proliferating ECs. The first phenotype represents the vast majority of normal, resting cells present in organisms, whereas the latter represents an angiogenic phenotype found in rapidly growing tumors.

We are also testing combinations of collagen, Matrigel, and other cell adhesion substrates. Quantitative assays of cell proliferation and qualitative assessment of cell growth are used to identify superior combinations of substrates.

Lastly, we continue to compare different endpoint assays or endpoint measures. For example, some bulk biochemical assays for apoptosis (e.g., Western blot) are appropriate for some large-scale irradiations, but for microbeam studies we can only analyze 3-5 orders of magnitude fewer cells and must use primarily histochemical techniques. For example, the literature has been a guide but surprisingly, in microbeam experiments, events have occurred much more rapidly than would have been predicted, thus we have had devote time optimizing timepoints and have had to delay the more sophisticated mechanistic experiments for future runs.

TECHNICAL PROGRESS AND RESULTS:

Cell culture experiments have been initiated in the investigators laboratory in the Medical Department (Bldg. 490). Notably, two runs have been completed at BNL's National Synchrotron Light Source (NSLS). Figure 1 depicts results from the first pilot study done at beamline X17B in May 2000 (***see Figure 1 on attached page***). Planar X-ray microbeams (170 keV) of 27 μm width were applied to confluent EC monolayers at various doses (0.5 - 40 Gy). To put this scale in a biological context, depending on cell density, an EC in a monolayer has a diameter of about 16-22 μm. A second run in July 2000 was done at a different beamline, X15B at 12 keV utilizing varying microbeam widths and doses (3-40 μm, 3-120 Gy). Results from these runs prove the concept that cell EC cultures are suitable for the work intended. In November 2000, we will have beamtime again at X17B in which biologically mechanistic issues can finally be addressed (e.g., up- or down-regulation of transcription factors such as c-jun and phospho-jun, threshold of irradiated gap size before the EC proliferative response is triggered, etc.)

Accomplishments in FY 2000 to date have consisted primarily of pilot studies. In the case of work at the NSLS, very basic things needed to be (and have been) worked out (e.g., constructing a sample holder, devising ways to prevent the chamber slides from leaking during and after irradiation, etc.).

In the coming period (FY2001), we will continue this work but with EC cells which have been differentiated to a microvascular phenotype by means of a cocktail of growth factors. We will also initiate co-cultures with astrocytes in order to model the BBB. Much of the basic tests we have completed in the previous period will form the basis for the upcoming work.

LDRD FUNDING:

FY 2000	$ 82,633
FY 2001	$100,000
FY 2002 (budgeted)	$100,000

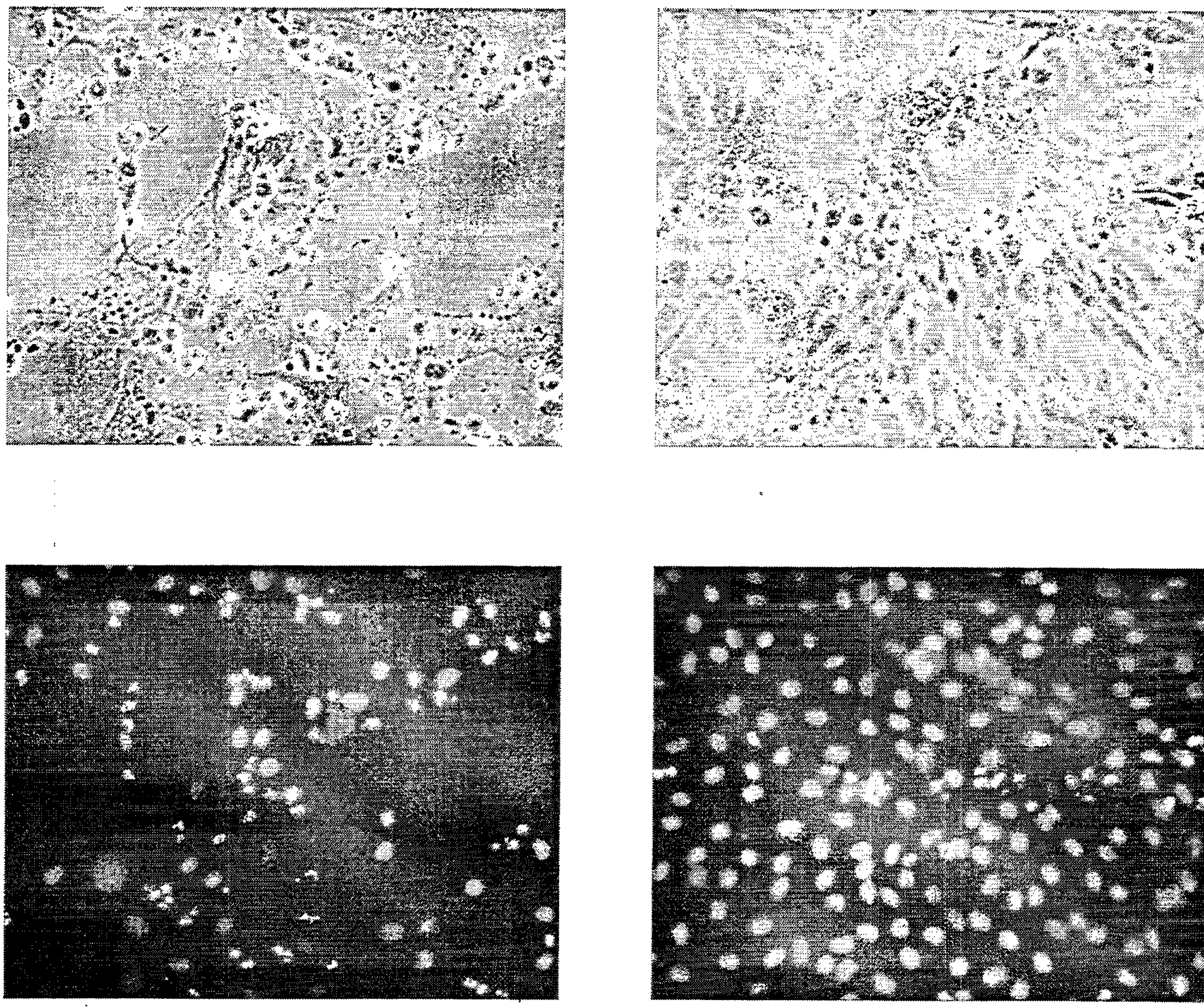


Figure 1. Endothelial cell monolayers, 6 hours after x-ray irradiation (170 keV), at the X17B beamline of the National Synchrotron Light Source, Brookhaven National Laboratory, NY. The dose applied to each was 24 Gy ($\approx LD_{75}$). *Left panels*: Conventional wide-beam x-rays cover the entire cell culture. *Right panels*: A single 27 μm wide microbeam horizontally traversing the entire cell culture. *Upper panels*: Brightfield phase contrast illumination. Rounded, phase bright cells above the plane of the monolayer are undergoing apoptotic death. *Lower panels*: Microscope fields identical to the panels above but under u.v. illumination, show condensed and fragmented bis-benzamide-stained nuclei indicative of apoptosis. (Peña & Dilmanian, unpublished results).

Investigating Surface Chemical Reactions and Kinetics from Atomic to the Nano Scale

J. Hrbek *00-35*
J. Larese

PURPOSE:

The goal of this project was to use tunneling microscopy and spectroscopy for the exploratory studies of surface chemical reactions with atomic resolution. Successful completion of this project was to enhance the BNL competitiveness in an anticipated DOE call for proposals in nanoscience.

APPROACH:

Use recently acquired UHV Variable Temperature Scanning Tunneling Microscope (STM) for studies of surface chemical reaction on single metal surfaces, surface defects of metallic and bimetallic model catalysts and their effect on chemical reactions, and reactivity of supported metal clusters relevant for catalysis.

TECHNICAL PROGRESS AND RESULTS:

State-of-the-art STM delivered in January was fully tested during February and March 2000. Procedures for strain metal deposition and reproducible tunneling tip etching were developed in collaboration with a visiting scientist from Sandia. Additional UHV equipment including quadrupole mass spectrometer, ion sputtering gun, electron beam metal deposition source, and LEED/Auger system were installed and tested. Search for RA was initiated in March after successful testing of the instrument.

LDRD FUNDING:

FY 2000	$48,849

The Structure of Membrane Proteins: Monolayers and Thin Films

Ben Ocko *00-40*
Dieter Schneider

PURPOSE:

To investigate the structure, oligomeric state, and interactions of membrane integral proteins by surface x-ray scattering techniques with the twin goals of developing new methods for obtaining structural information and to obtain fundamental information on the nature of protein membrane interactions. By varying the protein to membrane component concentration, detailed information can be obtained on the structure and on the protein-membrane interactions. An important aspects of our studies is to map out the phase behavior of membrane proteins as function of multiple environmental parameters including temperature, vapor pressure, surface pressure, solution phase conditions (salt, pH, etc.) and lipid terminal group interactions. These environmental conditions will provide for control of the internal protein conformations, and we will try to correlate these internal conformations with biological activity.

APPROACH:

The Physics Department X-ray Scattering Group has a significant effort devoted to understanding the structure of liquid/vapor interfaces and maintains Liquid spectrometer at the NSLS and APS to carry out these studies. Langmuir monolayers (monolayer film on a liquid subphase) provide an ideal environment for studying biological membranes. The molecular area and surface pressure can be accurately controlled which provides a degree of freedom not available in the bulk. In addition, the surface provides preferential alignment. Our approach is to use x-ray reflectivity and grazing angle diffraction to study the adsorption of integral membrane proteins.

TECHNICAL PROGRESS AND RESULTS:

In FY 2000, investigations of the adsorption of an 81 amino acid integral membrane protein encoded by the HIV-1 genome (Vpu) and synthetic proteins on phospholipid monolayers were carried out in collaboration with Kent Blasie's group at the University of Pennsylvania. In addition, studies of Langmuir monolayers of saturated and unsaturated fatty acids, both single component and mixtures were initiated. Initial studies of the adsorption of poly-L-lysine on a phospholipid monolayer were initiated. In addition, a specialized x-ray Langmuir trough was designed and ordered in April, 2000, and delivery is expected in December. This project has been on hold since August since our previous x-ray trough (on loan) was returned Vpu is an 81 amino acid integral membrane protein encoded by the HIV-1 genome with a N-terminal hydrophobic domain and a C-terminal hydrophilic domain. It enhances the release of virus from the infected cell and triggers degradation of the virus receptor CD4. Langmuir monolayers of mixtures of Vpu and the phospholipid 1,2-dilignoceroyl-sn-glycero-3-phosphocholine (DLgPC) at the water/air interface were studied by synchrotron radiation-based x-ray reflectivity over a range of mole ratios at constant surface pressure and for several surface pressures at a maximal mole ratio of Vpu/DLgPC. At relatively high surface pressures, the amphipathic helices of the cytoplasmic domain lie on the surface of the phospholipid headgroups, and the hydrophobic transmembrane helix is oriented approximately normal to the plane of monolayer within the phospholipid hydrocarbon chain layer. At maximal Vpu/DLgPC mole ratio, the tilt of the transmembrane helix with respect to the monolayer normal decreases with increasing surface pressure, and the conformation of the cytoplasmic domain varies substantially with surface pressure.

Grazing incident angle diffraction studies were carried out on a stearic acid monolayer and for a monolayer composed of a 1:1 mixture of stearic and elaidic acid. GID data is shown in the figure for an average surface pressures of ~8 mN/m for both monolayers. In the case of stearic acid this corresponds to a coverage of ~22 Å2/molecule and for the mixed monolayer this corresponds to a coverage of ~30 Å2/molecue. The diffraction pattern with the higher wave-vector peak on the L=0 axis and the lower peak off the L=0 axis is characteristic of orthorhombic packing with a nearest-neighbor tilt and an area per molecule of about ~22 Å2, determined from the lattice constants in agreement with the area obtained from the isotherm. For both samples as the surface pressure is increased, the off-axis peak position decreases corresponding to a smaller tilt. At sufficiently high surface pressure ~30 mN/m only a single peak is observed, corresponding to an untilted phase. The structure of mixed elaidic and stearic acid monolayer films exhibit the same GID patterns at the same surface structure, albeit at different molecular areas. This strongly suggests that the two components have phase separated where the stearic acid regions are ordered and the elaidic acid regions are disordered. These results are in contrast to the results of Fehrer that found mixed monolayers. If the two components had indeed mixed to form an ordered structure, then the molecular area would have been closer to 30 Å2/molecue and not the value of 22 Å2 /molecule calculated from the GID pattern. Subsequent Brewster Angle Microscopy studies provide support to our findings of phase separation.

In addition to the fatty acid studies, we initiated studies on the adsorption of poly-L-lysine, a protypical cationic protein, at the surface of a phosphatidylserine monolayer deposited on a phosphate buffer subphase (in collaboration with Stuart McLaughlin at Stony Brook). The very cationic protein should strongly bind to the acidic lipid, however, we did not observe any change in the surface normal density profile after the addition of the protein.

This project does not involve animal vertebrates on human subjects.

SPECIFIC ACCOMPLISHMENTS:

B.M. Ocko and M. Kelley, Phase Separation in Langmuir Monolayers, Stearic and Elaidic Acids (NSLS Abstract, 2000) S. Zheng, J. Strzalka, C. Ma, J. Opella, B. M. Ocko, and J.K Blasie, Structural Studies of the HIV-1 Accessory Protein VPu in Langmuirs, Monolayers, Synchrotron X-ray Reflectivity, J. Biophysics (accepted).

X-ray Studies of Maquette Peptide Monolayers, I. Reflectivity and GID at the Air/Water Interface, J. Strzalka, X. Chen, C.C. Moser, P.L. Dutton, B.M. Ocko, and J.K. Blasie, J. Biophysics (accepted).

Reorientation of the alpha-helical synthetic peptide ZnPPIXBBC16 in the Langmuir Monolayer, A. Tronin, J. Strzalka, X. Chen, P.L. Dutton, B.M. Ocko, and J.K. Blasie, Langmuir (submitted).

LDRD FUNDING:

FY 2000	$16,566
FY 2001 (budgeted)	$50,400

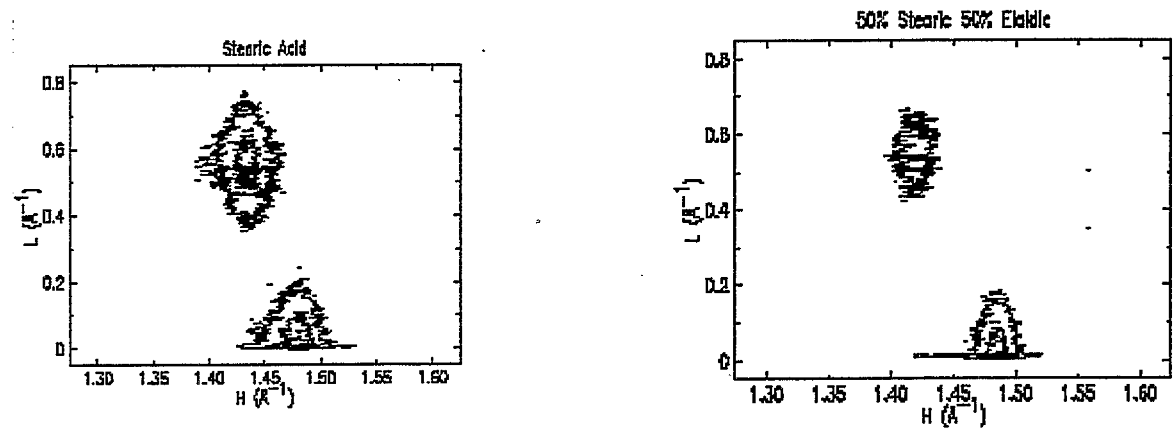


Figure: Grazing incident angle diffraction pattern from a monolayer of stearic acid (top) and a 1:1 mixture of stearic and eladic acids, both at~8 mN/m at 15 °C. The similar patterns suggest phase separation.

Mobile Agent Based Monitoring of Distributed Computing Systems

Richard Ibbotson *00-42A*

PURPOSE:

The goal of this project is to demonstrate the feasibility of using Java-based mobile agents, a new software technology, to produce a platform-independent, highly flexible tool set capable of measuring end-to-end performance for distributed computing systems in a wide variety of metrics. If successful, this approach will be used for the basis of a monitoring system for the RHIC Computing Facility.

APPROACH:

A Java mobile agent system will be selected and used to develop a template for a computing facility performance-measuring instrument. An overall clearing house for instruments and their reports will be established and the feasibility of using agents as instruments demonstrated by instantiating and operating one or more such instruments.

TECHNICAL PROGRESS AND RESULTS:

In FY 1999, a specific implementation of Java mobile agent technology was selected for conducting this demonstration. The framework for automatic instantiation, dispatch and receipt of specialized agents was developed, and a relational database schema was developed to contain the reports and byte-code for the agents.

In FY 2000, a template for the instruments based on these agents was developed, and five sample agents were created. Each agent was designed to gather system-specific information: write- and read-throughput for network-mounted file-systems, load-average on a specific host, network traffic over specific interfaces and statistical information for HPSS tape drives. A web-based report-generation system was developed which allows selection of test-specific parameters and hosts and provides graphical representations of the requested data.

During FY 2000, the sample mobile agents described above were used to regularly perform measurements on between 1 and 50 hosts, depending on the specific agent. Certain specific elements of the design of the Aglets package created problems with the scalability of the architecture; these problems were overcome by altering the security scheme that prevents unauthorized mobile agents from entering the system.

In FY 2001, the scale of the system will be increased, and the feasibility of scaling the system to the order of 200 computers will be tested. Based on experiences with the system so far, the response of the MySQL database may be the limiting factor in the system. In this event, other relational databases will be evaluated.

SPECIFIC ACCOMPLISHMENTS:

"A Mobile-Agent Based Performance-Monitoring System at RHIC" presented at CHEP 2000. (Computing in High-Energy and Nuclear Physics)

LDRD FUNDING:

FY 2000	$144,871

Demonstration of Advanced Commercial Ethernet Technology

Terrance Healy *00-42B*

PURPOSE:

The goal of this project is to establish that a complete set of next generation commercial Ethernet components exists and that they are mature enough to make feasible a production level very high performance Local Area Network (LAN) based on them. If successful, this approach will be used as the basis for the local area network of the RHIC and US ATLAS Computing Facilities.

APPROACH:

Contrary to predictions four years ago that Asynchronous Transfer Mode (ATM) technology would dominate the future of Local Area Network (LAN) evolution, a variety of innovations to the Ethernet standard have appeared and now seem destined to play a significant role in the LAN market for the foreseeable future. While of modest and continuously decreasing cost, advanced commercial Ethernet products seem to offer performance comparable to very high performance interconnect options including ATM and High Performance Parallel Interface (HIPPI), both of which are very much more costly. A set of products was to be identified and acquired via loan or purchase. This set would then be integrated into one or more systems and tested for interoperability, functionality, performance and reliability.

TECHNICAL PROGRESS AND RESULTS:

In FY 1999 target products, vendors and platforms were identified, equipment acquired and initial test undertaken. Work done in FY 2000 has demonstrated that certain of these technologies are mature enough for production use, in particular Gigabit Ethernet interfaces and switches and also Virtual Local Area Network (VLAN) capable switches. There remains significant interoperability and stability problems with the versions of extended frame, so called "Jumbo" frame, Ethernet and physical line trunking technologies tested. These are, therefore, regarded as not mature enough products to be use other than in areas of particular need and then with significant caution. No testing of 10 Gigabit Ethernet has yet been done.

Advancing technology has overtaken this project. The advanced technologies being studied are now beginning to be widely deployed in production operation. While continued R&D in this area is required, it can no longer be properly regarded as innovative so further LDRD support for this work will not be requested. It is clear the evolution of Ethernet, not ATM technology, will dominate the LAN market at least in the near and mid-term, and this is now the basis of the RHIC and US ATLAS Computing Facilities LAN's.

LDRD FUNDING:

FY 2000	$100,000

Cyber Security for Wide Area Distributed Collaborations

Shigeki Misawa *00-42C*

PURPOSE:

The goal of this project is to establish the feasibility of an adiabatic approach to supplying adequate cyber security to a large computer facility supporting a large Wide Area Network (WAN) connected community without extensive disruption to the users of that facility. The conflict between cyber security concerns and the access needs of wide area distributed collaborations pose a major problem of particular importance to the current and next generation of large High Energy and Nuclear Physics experiments.

APPROACH:

The demonstration architecture includes secure shell (ssh) gateways, application proxies, substantial host service restriction and monitoring and the use of a firewall to monitor and control overall access. We will employ dedicated servers for particular functions to allow for a high level of system specific security and in general to produce better performance, higher reliability, and easier system administration.

TECHNICAL PROGRESS AND RESULTS:

In FY 2000, two machines to be used as system gateways were purchased and configured to support only ssh access, an additional machine was configured to supply proxy file transfer protocol (ftp) service. In addition, a firewall was purchased and installed and filtering rules for it defined. Various host monitoring and access control packages were acquired and configured on the demonstration systems. Iterative feed back from the users of the demonstration systems was used to optimize trade offs between security and ease of access and use as security was increased. While the introduction of various of these technologies involved some degree of re-education of the user community, it has proven to be possible to arrive at a very significantly improved cyber security stance without major disruption. After approximately one year of evolution the demonstration system was able to support a relatively large group of users in an environment in which no clear text password were used on the network and where external access was wholly limited to gateway systems which by virtue of their functional specialization could be made very secure.

While the level of security and user acceptance achieved by this project has been very high, the project has been overtaken by much more draconian security measures being deployed site-wide by the Laboratory's Information Technology Division. These measures introduced more abruptly with less user feedback have resulted in major user disillusionment with cyber security and have arguably resulted in very marginal improvement relative to the more adiabatic approach.

LDRD FUNDING:

FY 2000	$100,000

Data Mining Strategies for HENP Experiments

Bruce Gibbard *00-42D*

PURPOSE:

The goal of this project is to study the feasibility of using simple data mining strategies in place of more sophisticated but costly to implement approaches. It is important to understand if there are regimes in which simpler, less expensive and more easily deployed data mining strategies might produce comparable or perhaps even superior performance to heavier weight systems.

APPROACH:

There can be dramatic differences in the amount of sophistication and effort that go into the systems that support High Energy and Nuclear Physics data mining. Two different strategies have been proposed with the goal of extracting selected data subsets from Petabyte scale data sets located on tertiary storage. One involves the correlation of relatively complex Standard Query Language (SQL) like data queries at the object container level within a data store. Such a system has been developed over the course of the last three years under a DOE Computational Grand Challenge (CGC) initiative. The second strategy involves the correlation of simple file level requests. This second strategy is to be prototyped and metrics developed to assess its performance relative to the CGC approach above and to do a cost benefit comparison of the two approaches.

TECHNICAL PROGRESS AND RESULTS:

In FY 2000, the simpler data mining strategy was prototyped. This strategy requires the user to know the files in which desired data is to be found. Given this list of files it optimized the order in which those files were retrieved based on knowledge of the particular tape on which each file was located and its position on that tape. This significantly reduced the number of tape mounts and the amount of searching on each tape. This system was exercised in Mock Data Challenge exercises and with real RHIC physics data taken late in FY 2000. The CGC developed system was also exercised. The cost of the more sophisticated CGC system in terms of technical effort is an order of magnitude more (~10 FTE-years versus <1 FTE-year). The fact that these two systems were used by different experiments made it very difficult to define effective common metrics of performance. It was, therefore, not possible to do a quantitative comparison of the relative cost benefit of the two systems.

The apparent level of satisfaction shown by users of the two systems was comparable. Given that satisfaction as a metric one might conclude that the simpler system is more cost effective. However, the CGC system clearly has a higher level of functionality and, therefore, could be of more general use which would distribute its development cost across multiple High Energy or Nuclear Physics experiments, thus ameliorating its higher cost. At this time more general adoption of the CGC system remains to be demonstrated. While failing to quantify the relative cost/benefit ratio of high and low development cost systems, this project clearly demonstrated the useful role of low development cost data mining efforts.

LDRD FUNDING:

FY 2000	$100,000

Parallel Linux Systems

Thomas Throwe *00-42E*

PURPOSE:

The goal of this project is to investigate an innovative concept for performing parallel system administration in a manner that scales well with the number of computers and allows for customization based on hardware configuration and individual problem type. This is important today where large arrays of commodity computers (typically Intel processor based) are being run using the Linux operating system to perform computations previously performed by a small number of super computer or large-scale symmetric multiprocessor systems each requiring the maintenance of only a single copy of the operating system.

APPROACH:

The approach is to initially ***clone*** a prototype computer's operating system image across the Local Area Network into each member of an array of computers. Each computer then uses a set of database-maintained scripts to customize its own operating system image before doing an additional reboot to its final working operating system configuration.

TECHNICAL PROGRESS AND RESULTS:

In FY 2000, a version of this system was developed that makes use of the database management product, MySQL, to maintain the configuration characteristics of over 400 Linux systems. These systems came from multiple hardware vendors (up to five) and included 10's of different hardware configurations (disk, memory, numbers, and speeds of CPU's). These systems were configured with several different software configurations based on various types of uses by each of five different experimental collaborations.

The system has proven to be very effective. It allows one to rapidly reallocate machines between users and uses. It also allows one to upgrade a subset of the machine to a new operating system or other software configuration rapidly with minimal human effort and a very high level of reliability. In general the system allows for the required effort to scale only as the number of different configurations and to be largely independent of the number of machines of any particular configuration. This is of course critically important to large High Energy and Nuclear Physics projects where the required computing power is obtained by configuring processing farms including 100's of functionally identical machines for individual experiments.

SPECIFIC ACCOMPLISHMENTS:

"RHIC Computing Facility Processing System" presented at CHEP 2000. (Computing in High-Energy and Nuclear Physics)

LDRD FUNDING:

FY 2000	$100,000

Understanding Pathways of Ubiquitin Dependent Proteolysis

Maria Bewley *00-43*

PURPOSE:

A biological cell is a complex set of machines that work in harmony, yet little is understood about its inner workings. A key first step in addressing this problem is to study simpler multi-component biological systems, and this is the overall goal of this research. Current understanding of the simpler systems is often incomplete because, typically, individual proteins are studied in isolation rather than in the context of their biologically relevant complex. In order to address this problem, structural studies must be made on a system as a whole. Two examples of such systems that have been chosen for further study are the pathway by which DNA double strand break (DSB) repair occurs in mammalian cells, and the secondary system is the electron transfer pathway of fatty acid biosynthesis and nitrate reductase (NR). The first pathway is important because unrepaired DNA damage leads to chromosomal errors and cell death. The second pathway is important in understanding a basic principle in cellular function.

APPROACH:

Addressing the question of DSB repair is a huge undertaking that can only be successful if a large number of approaches are tried. Therefore, in a collaborative effort with Carl Anderson, Paul Freimuth and John Flanagan, we are each addressing a distinct aspect of this pathway. This LDRD is using a "divide and conquer" strategy to obtain structural information about the proteins involved. Briefly, domains of DNA-PK will be identified using a combined bioinformatics and controlled proteolysis approach. Domains identified in this way will be overexpressed initially in *E.coli* using commercially available expression vectors that incorporate a purification tag and any soluble products purified utilizing the tag. Pure protein will then be crystallized and it's structure determined using the Multiple Anomalous Dispersion (MAD) technique. It is not uncommon that mammalian protein domains do not express as a soluble entity. In such cases, either attempts to refold the protein or alternative expression systems such as insect cell lines will be investigated.

Addressing the question of electron transfer, by comparison to DSB repair, is a more modest undertaking. The reduction of nitrate to nitrite is catalyzed by the enzyme nitrate reductase (NR). It contains three domains, a flavinadeninindinucloetide (FAD)-binding domain, a cytochrome, and a molybdopterin. The electron flow during catalysis follows the scheme substrate-> FAD -> cytochrome -> Mo -> nitrate. In a different system, fatty acid desaturation, involves the transfer of electrons from b5 reductase (B5R)-bound substrate to cytochrome b5. Clearly, communication between the domains and thus protein:protein interactions will play a key role. In collaboration with Dr. M. Barber at the University of South Florida, who provides the protein samples, I am using protein crystallography to understand this transfer process.

TECHNICAL PROGRESS AND RESULTS:

DSB-repair: In order to obtain structural information about DNA-PK and its partners, domain boundaries have to be identified within the sequence and these regions cloned, overexpressed, purified and crystallized. In additon, purified protein provides tools to other members of the consortium to quantitate such interactions. We have made predictions about the location of domain boundaries using bioinformatics tools that are available on the internet. The 3128 DNA-PK catalytic subunit has been divided up into putative domains. In addition, domains of proteins that are known to interact with DNA-PK have also been identified. Expression of such domains is usually initially tested in prokaryotic expression systems, since they are relatively inexpensive, robust, and fast. Each of these domains have been sub-cloned into a pET expression vectors and transformed into *E.coli* cells. Approximately half of the clones overexpress proteins, however, none are soluble (a requirement for crystallization). In cases such as these it is common either to refold the protein, attach a retargeting or solublizing tag, or transfer into prokaryotic expression systems. We have tried a number of these approaches.

For FY2001 and in collaboration with Dr Freimuth, the expression vector that he has developed will be used to attempt to produce soluble protein. In addition, in collaboration with Dr Flanagan, other expression systems will be pursued; and when soluble protein is obtained, the tools developed by him will be used to show that a biologically relevant complex has been formed.

Electron transfer: Microcrystals of the cytochrome b5 domains for rat and spinach have been obtained. My collaborator has overexpressed and purified fusion proteins that contain an active complex of the FAD and cytochrome domains.

In FY2000, the crystal structures of rat B5R and spinach nitrate reductase have been solved to 2.0Å and 2.4Å resolution, respectively. The second structure has been solved in the presence of FAD (at 2.4Å resolution) and additionally in the presence of a substrate analogue, ADP-ribose (to 2.7Å resolution).

For FY2001, an atomic resolution model will be sought. Crystallization screens will continue in order to obtain diffraction quality co-crystals of the FAD domain in complex with the cytochrome b5 domain. Based on the structures solved, structural characterization of mutants will be performed

This project does not involve any animal experiments or research on human subjects.

SPECIFIC ACCOMPLISHMENTS:

DSB-repair: None

Electron transfer: Manuscripts for publication in peer-reviewed journals are in preparation for the newly solved structures. The running title for the first is "*Crystal structure and biochemical characterization of rat b5 reductase at 2.0Å resolution*" and corrects a previously incorrect model solved by others and now provides a starting model that is consistent with the biochemical data. The running title for the second is "*Structrual plasticity in the FAD of nitrate reductase suggests a mechanism for the first stages of electron tranfer*" The structures show different conformations for the FAD domains and suggest a model for substrate binding.

LDRD FUNDING:

FY 2000	$244,247
FY 2001 (budgeted)	$215,000

Structural Characterization of DNA-PK, a Human DNA Double-Strand Break Repair Protein

John M. Flanagan 00-44
Carl Anderson

PURPOSE:

The goal of this project is to determine high-resolution structures of the DNA repair components involved in Double Strand Break Repair (DSBs). DSB are produced by ionizing radiation and their efficient and faithful repair is essential since the presence of a single unrepaired DSB can result in cell death, or in mammals, cancer. At present little is known about the detailed mechanism of DSB repair, although this process has important mechanistic implications for modeling the effects of low doses of radiation on cells and in treating human cancers. To date, mechanistic studies of the pathways for DSB repair have suffered from a lack of high-resolution structures for their components. We will focus on obtaining functional complexes containing DNA-PK_{cs} a component of the non-homologous end joining pathway for DSB repair that are suitable for crystallographic structure. DNA-PK_{cs} forms a functional hetero-oligomeric complex with two other proteins Ku70K80.

APPROACH:

Non-homologous End Joining (NHEJ) is the major route by which DSBs are repaired in mammals. A number of laboratories, including that of CoPI Carl Anderson, have begun to identify specific components in this pathway including DNA-PKcs, Ku70Ku80. However, due to the complexities of the system, and the fact that most of the components are not available in sufficiently large quantities, our understanding of how DSBs are repaired by this process is still incomplete. With our collaborator Dale Ramsden at the University of North Carolina, we have made strides in obtaining sufficient quantities of DNA-PK_{cs}, Ku70, and Ku80, three of the key components of NHEJ for mechanistic and structural studies. These proteins form a complex that binds to the free DNA ends at DSBs and is thought to be one of the first steps in identifying broken DNS ends and then recruiting the other components of the repair complexes to these sites. The availability of these reagents has allowed us to prepare defined and stable complexes that are suitable for crystallization trials. Our initial trials will focus on a ~700kDa complex containing DNA-PK_{cs}-Ku70Ku80-DNA. This is a relatively large complex for X-ray crystallography, however, the recent successful determinations of the atomic resolution structures of the ribosome and the *E. coli* RNA-polymerase suggest that it is well within the current capabilities of the beamlines at the NSLS.

TECHNICAL PROGRESS AND RESULTS:

During FY 2000, we successfully purified the Ku70Ku80 components from the insect Baculovirus expression systems. These studies clearly demonstrate the feasibility of obtaining 5-10mg of homogeneous Ku70Ku80 for crystallization trials. Our initial biochemical studies with the Ku70Ku80 complex indicate that complex stability is greatly enhanced by the presence of DNA-PK_{cs}, and thus it seems likely to us that co-crystallization efforts will be more likely to yield diffraction quality crystals. Currently there is no expression system for intact DNA-PK_{cs}, however, previous studies in Carl Anderson and other laboratories indicate that DNA-PK_{cs} is a relatively abundant protein in mammalian tissues. However, our experience is that during purification of the protein from these sources the majority of DNA-PK_{cs} is lost and that a significant fraction of the remainder is proteolytically nicked by an endogenous protease. During the second half of FY2000 we began pilot studies aimed at obtaining larger quantities of extremely pure DNA-PK_{cs} from human placenta or HeLa cells in tissue culture. Through these efforts we have identified a rapid high-yield procedure to obtain intact DNA-PK_{cs}. Based upon these results it is likely that ~5mg of the enzyme can be obtained from 100L of HeLa cells. In addition to the proposed crystallographic studies the availability of these quantities of DNA-PKcs and Ku70Ku80 has allowed us to begin in parallel mechanistic studies. Using purified components we have begun a thermodynamic analysis of complex formation between DNA ends and Ku70K80 alone and in their ternary complex with DNA-PK_{cs}.

The studies described above form the basis for our crystallization experiments of the DNA-PKcs-Ku70Ku80-DNA complex. In addition, they have opened several new lines of inquiry that are being followed: 1) Kinetic analysis of complex formation; 2) examination of the role of DNA-PK in recruiting other components of the NHEJ repair apparatus. Our current hypothesis is that the DNA-dependent protein kinase activity of DNA-PK_{cs} will play a role in regulating complex formation and perhaps the activities of specific repair components.

SPECIFIC ACCOMPLISHMENTS:

As a result of the initial studies we have attracted new DOE funds (Contract No. DE-AC02-98CH10886). The studies supported by continuation of this LDRD are aimed at attracting additional funding most likely from the National Institutes of Health.

LDRD FUNDING:

FY 2000	$44,132
FY 2001 (budgeted)	$95,200

New Protein Expression Tools for Proteomics

Paul I. Freimuth *00-45*

PURPOSE:

Our technical objective is to optimize the folding of recombinant proteins into their native, biologically active conformations in *E. coli*, a bacterium which can synthesize proteins in quantities sufficient for biophysical analyses such as X-ray crystallography. Protein folding *in vivo* is catalyzed by chaperones, and it is thought that the absence of appropriate chaperones accounts for the misfolding of many foreign proteins in bacterial cells. Other groups have attempted to solve this problem by modifying bacterial cells to express appropriate chaperones, with limited success. We are investigating whether recombinant proteins themselves can be modified to promote their folding in the context of normal bacterial cells. Our study will provide insights into the basic mechanisms of protein folding *in vivo* and may lead to improved methods for protein production that would be of direct benefit to the BNL Initiative in Proteomics.

APPROACH:

Background. In studies leading to this LDRD project, we observed that a human membrane protein (CAR) which usually misfolds in *E. coli* could fold properly if the protein carboxy-terminal end was fused to a particular short peptide. This effect is specific, since folding of the protein was not rescued by fusion to other peptides of similar length but different sequence. We formulated the hypothesis that this C-terminal peptide mediates folding either by substituting for human chaperones that normally fold CAR or by enabling *E. coli* chaperones to interact productively with this human protein.

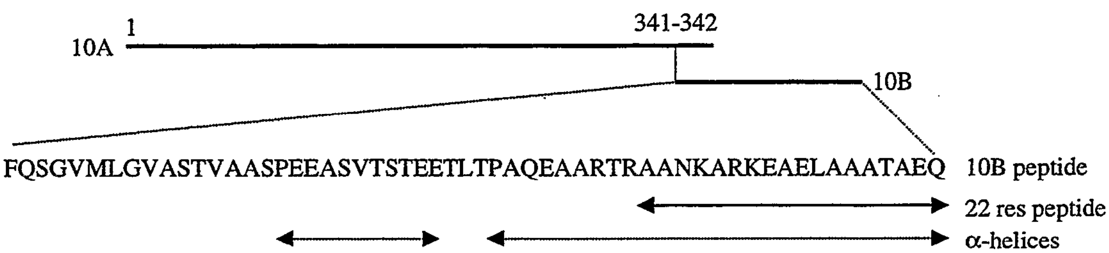
Scope. The scope of our project is: (1) to characterize features of this C-terminal peptide that are necessary for its protein folding activity within bacterial cells, (2) to determine the generality of this folding activity and the rules governing what types of proteins can or cannot be folded by this peptide, and (3) to determine whether this peptide can promote renaturation of misfolded proteins *in vitro*.

Methods. To characterize features of the peptide necessary for its protein folding activity, we will analyze the peptide sequence to predict its secondary structure and its similarity to other known peptide sequences. Then, mutations will be designed to disrupt specific features suggested by these analyses. To assess the generality (universality) of this peptide-mediated folding approach, we will fuse the peptide to a set of yeast proteins previously selected in the BNL Proteomics Initiative as targets for X-ray crystallographic analysis. In the absence of the peptide all of these proteins misfold and precipitate during synthesis in *E. coli*. To determine whether the peptide can mediate renaturation of misfolded proteins *in vitro*, we will characterize renaturation reactions in the presence and absence of added synthetic peptide.

TECHNICAL PROGRESS AND RESULTS:

Synthetic peptide: The following 22 residue peptide was synthesized commercially (Research Genetics, Inc.): (acetyl-cysteine)-LEDPAANKARKEAELAAATAEQ. An amino-terminal cysteine residue was added to introduce a reactive sulfhydryl group for coupling to beads or to other supports. The peptide was coupled to SulfoLink beads (Pierce) and added to protein renaturation reactions; however, it did not improve yields of refolded protein. The peptide also was coupled to activated KLH, and a rabbit was immunized with the peptide-KLH conjugate (performed by Cocalico Biologicals, Inc.) to raise peptide-specific antibodies.

Peptide features: The 22 residue peptide is derived from the carboxy-terminal end of the phage T7 gene 10B protein, a derivative of the major capsid protein 10A which arises from a shift in translational reading frame as shown in the following diagram.



The 10B peptide is exposed on the surface of the T7 capsid and is predicted to contain 2 α helices, but its function has not been elucidated. CAR was fused to the entire 57 residue 10B peptide and to 10B residues 18-57. Both peptides completely rescued the folding of CAR, whereas the original 22 residue peptide (10B residues 40-57) was only partially active. These results suggest that both predicted α-helices may be required for full activity of the 10B peptide.

Universality of approach. A set of 7 yeast proteins was fused to the 22 residue peptide. Folding of 2 of these was rescued to >50%, while another 2 were rescued to about 25%. Folding of the remaining 3 proteins was not measurably affected by the peptide. In future studies we will determine whether the full-length 10B peptide further improves the folding of these proteins as it did for the CAR test protein. The full-length peptide will be mutagenized to determine whether one or both of the helices are required for its folding activity. Finally, the peptide-specific antibodies will be used for biochemical analysis of the folding mechanism.

SPECIFIC ACCOMPLISHMENTS:

A manuscript "Fusion to a phage T7 gene 10B-derived peptide enhances protein folding in *Escherichia coli*" is in preparation. A patent application "*Cis*-acting peptide chaperone" also is in preparation.

LDRD FUNDING:

FY 2000	$ 41,698
FY 2001	$111,000
FY 2002 (budgeted)	$111,000

High-Throughput Structure Determination for the Human Proteome Project

F. William Studier *00-47*

PURPOSE:

Structural genomics is the systematic determination of 3-dimensional structures of proteins to survey the range of protein structures and functions found in nature. The information and tools generated by structural genomics will provide a framework for understanding biochemical functions and interactions of the proteome of any organism whose genome sequence is known. This capability will further DOE aims such as understanding effects of ionizing radiation and pollutants on human health and harnessing biological processes for bioremediation or carbon fixation. This project addresses a need for informatics, database, and computational support for structural genomics in three areas: 1) access to and manipulation of information about proteins found in public databases and web sites; 2) a database and web interface for managing experimental data and work flow for a consortium for high-throughput protein structure determination; and 3) software to reduce the human effort involved in processing x-ray diffraction data from protein crystals to produce high-resolution protein structures.

APPROACH:

We are part of a consortium of scientists at five different institutions piloting high-throughput determination of protein structures, which requires the integration of a wide range of activities, including selecting protein targets; cloning, expressing, purifying and crystallizing the selected proteins; collecting diffraction data at synchrotron sources; processing the diffraction data to determine protein structures; and annotating and depositing structures in the Protein Data Bank. The need for informatics, database, and computational support was apparent from the beginning.

Informatics and database development at BNL is directed by Dawei Lin, assisted by a postdoctoral associate and summer students. The approach is to design systems that gather and organize information from a wide range of public sources, facilitate the capture of locally generated experimental data, and provide status reports needed to manage the workflow. Web interfaces are used to enter data and display reports. Iterative interaction with experimentalists who are selecting protein targets and generating materials and data is crucial to the development of a system that effectively serves the needs of the consortium.

As the production of protein crystals accelerates, the need to streamline the process of obtaining an accurate structural model from x-ray diffraction data becomes increasingly important. Integration and improvement of multiple programs used by crystallographers in the process of model building could potentially reduce direct human involvement in determination of a protein structure from weeks or months to hours or days. Such advances will be essential for achieving the needed efficiency of high-throughput structure determination. Jiansheng Jiang is developing an integrated pipeline of computer programs most commonly used in the structure determination process and is exploring computational approaches to reducing the demand for judgments by a skilled crystallographer in building the amino-acid chain into the electron density map. He interacts with S. Swaminathan, the crystallographer who is directing structure determination for the structural genomics pilot at BNL, and with crystallographers who come to use the protein crystallography stations at the NSLS. In FY 2001, he will be assisted by a postdoctoral associate.

TECHNICAL PROGRESS AND RESULTS:

The Structural Proteome Database (SPD) is an evolving database and associated set of computational tools to facilitate the collection and organization of data needed for the selection of protein targets for structure determination and annotation of newly determined structures. A prototype web interface was implemented for testing and feedback from experimenters. The prototype SPD was used to select 90 targets for attempted structure determination from a set of 220 human proteins identified by a collaborator as being likely to have significant roles in the response of human cells to ionizing radiation. This information formed the basis for a successful application to DOE to determine structures of human proteins involved in radiation response.

The Internal Consortium Experiment Database (ICEdb) is an evolving database and associated web interface to collect and query the results of a great variety of procedures involved in obtaining proteins and determining their structures. A schema was developed through interaction with the biochemists and structural biologists who will rely on ICEdb to archive results and track the progress of experiments. A prototype web interface was implemented and the first web forms to deposit data were developed, concentrating initially on cloning and tests of protein expression and solubility (including images of gel electrophoresis patterns). Software was developed to extract information directly from the database into an organized report for posting progress on our publicly accessible web site www.proteome.bnl.gov.

A pipeline of programs used for protein structure determination was constructed and is now in beta release through the Automated Structure Determination Package (ASDP) web site http://vivaldi.bio.bnl.gov. A database of secondary structure elements was assembled from non-redundant protein structures in the Protein Data Base for use in developing automated model building.

Development of both SPD and ICEdb will continue in FY 2001 as will further development of the ASDP web site and exploration of other approaches for improving the automation of protein structure determination.

SPECIFIC ACCOMPLISHMENTS:

Information provided by the prototype SPD and ICEdb facilitated the development of successful applications to DOE for "Analysis of Human Proteins Induced in Response to Ionizing Radiation" and, as part of the New York Structural Genomics Consortium, to become a pilot center in the Protein Structure Initiative of the National Institute of General Medical Sciences. An invited presentation at the International Conference on Structural Genomics 2000, November 2-5, 2000, Yokohama, Japan, includes work supported by the LDRD. An abstract describing SPD was submitted for consideration for the RECOMB 2001 International Conference on Computational Molecular Biology, April 21-24, 2001, Montreal, Canada.

LDRD FUNDING:

FY 2000	$575,570
FY 2001 (budgeted)	$290,000
FY 2002 (budgeted)	$290,000

Design Study of a Solid Target for Spallation Neutron Sources

J. Hastings *00-49*

PURPOSE:

Modern spallation sources running at proton energies of order 1 GeV have mainly used plate targets with the coolant passing between the plates in the path of the proton beam. These targets have been very effective sources. They have even been considered for the next generation machines, SNS for example, but liquid mercury has been settled on as the target material of choice. There are two exceptions to this however, the proposed target for the second target station at ISIS and the target for AUSTRON, a 500KW facility proposed in Austria. These both propose to use solid targets. A solid target is also well matched to the properties of the AGS, specifically its high energy compared with conventional pulsed spallation sources. The project is aimed at the challenging task of designing an optimum target consistent with the 24 GeV proton energy and the desire to make a very bright neutron source.

APPROACH:

We have chosen to implement the idea of a solid rod target based on a concept that has been used successfully at CERN for their antiproton source and has the advantage that no cooling water is in the beam and the target is at the maximum possible density. The concept for the average power at CERN, 17 kW, has been proven to be very reliable. We have extended this to a target capable of the full average power of the AGS today, typically 100KW. If successful this prototype design and the detailed engineering analysis will be the important to the general field of spallation target development. The design procedure combines thermal analysis for the average power and transient analysis to ensure mechanical integrity for the peak pulse energy. The input data for these studies (energy deposition in the target and target assembly) is based on detailed calculations of the spallation process. These calculations are iterated and include as well the desire to make the target assembly passively safe against a loss of coolant failure.

TECHNICAL PROGRESS AND RESULTS:

The initial phase of the project has concentrated on developing the engineering tools, in particular the transient analysis, to permit a complete and detailed design of the target. To this end we have verified the LSDYNA results for a specific target geometry for which an analytic solution for the time evolution of the strain exists. We have also carried out preliminary thermal analysis to ensure that the decay heat (residual heating due to the decay of the activated target) does not melt the target for a loss of coolant accident. These calculations have been based on scaling the CERN design, optimized for antiproton production, to a design optimized for neutron production. In particular, we have assumed a tungsten target surrounded by a graphite interface and then inserted in a copper outer shell. The target length is 30 cm compared to 7 cm for the CERN design, and the diameter is 5 cm compared to 6 mm. These differences are dictated by the needs for a neutron source (length) and the significantly increased power (diameter). The next step is to iterate on this concept with the goal to minimize the diameter of the target assembly so as to increase the source brightness. Possible changes include removing the graphite interface layer.

In addition to the preliminary engineering studies, the needed modifications to the AGS beamline, C7, where the prototype target is to be fully tested have been started.

This project will continue in FY2001 during which time the design concept will be optimized as outlined above and a detailed design will be completed. The design will be reviewed prior to construction by an outside panel of experts and hopefully leading to construction starting in FY01.

SPECIFIC ACCOMPLISHMENTS:

Results of the code validation:

Paul A. Montanez, Peter Sievers "Validation of a Computer Code for Use in the Mechanical Design of Spallation Neutron Targets," Journal of Neutron Research, accepted for publication.

LDRD FUNDING:

FY 2000	$301,241
FY 2001 (budgeted)	$194,000
FY 2002 (budgeted)	$194,000

Remote Full Field Dynamic Optical Measurement of Structural Integrity

R. Hall 00-61
J. Taylor

PURPOSE:

A currently acknowledged crisis facing the nation is the aging of its infrastructure. Maintenance and modernization initiatives prove too costly, inspection techniques are inefficient, and at times ineffective, and there exist no realistic real time monitoring systems that can warn of incipient catastrophic failures. This project singles out these issues as related to heavy structures such as long-span roof supports, bridges and overpasses, and building facades. The goal of this research is to explore the feasibility of using a remote, non-contact sensor system capable of continuously monitoring and evaluating the conditions of complex structures under real life fatigue and corrosion.

APPROACH:

The research explores the phenomena that occur when an optically rough surface is exposed to a coherent laser beam. The reflected wavelets create a random interference pattern in the form of speckles. As the structure moves, so do the speckle patterns, which can then be correlated to the deflection and twist of the structure. The major challenges in this work will include:

1. The digitization of those random patterns and the development of advanced algorithms that correlate these data to actual structural movements and failure.

2. Application of the laser beam in a full-field mode that can be used to determine dynamic and vibrational deformation.

3. Compensation for atmospheric optical noise such as rain, snow, smog and thermal plumes.

4. Application of retro-reflective coatings on the structures of interest to enhance measurement sensitivity.

This research will lead to a full-scale proof of principle, demonstration of this innovative concept on a structure to be identified on the Lab site. If successful, this work can lead to enhance public safety, reduced traffic congestion, and support to DOE's smart buildings and industries of the future programs.

This year Dr. U. VonWimmersperg, Mr. R. Hall and a summer student from SUNY Stony Brook, Mr. J. Antonakakis along with consultation from Drs. E. Guan and F.P. Chiang of the Mechanical Engineering Dept. of Stony Brook represented the collaborators on this program.

It was decided to investigate the application of speckle interterometry to full field structural deflection and torsion under low loads. This required understanding of a simple full-scale beam structural response and the use of a low power laser transmitter and digital camera receiver. This research was based on earlier small-scale laboratory studies of modal shapes in a cylindrical shell performed by Dr. Chaing

TECHNICAL PROGRESS AND RESULTS:

The activities under this report cover the time interval from February 2000 through

July. A testing program was developed based on full-scale monitoring of a beam structure under loading from a mechanical shaker. The test apparatus consists of a low power He-Ne laser, a beam expander, a 512 x 480 CCD camera and a PC was assembled, setup and calibrated. Image processing software developed by the Stony Brook team was imported and evaluated for expansion and use in future experiments.

SPECIFIC ACCOMPLISHMENTS:

An informal internal report was written by the summer student, J. Antonakakis representing early thinking on, and calibration of the experimental setup. A Safety Assessment, 1.3.5 was submitted to begin the experimental work.

An invited paper was presented on the Smart Cities concept at the "Life Extension Technologies – Second International Workshop," September 27, 28, and 29, 2000, in Paris, France.

LDRD FUNDING:

FY 2000	$ 58,000

Muon Collider & Storage Ring Neutrino Beam Study

R.B. Palmer *00-93*

PURPOSE:

Brookhaven is playing a leading role in a DOE-funded collaboration studying the feasibility of muon colliders and muon storage ring based neutrino factories as future high energy facilities. This LDRD proposal has several components related to, but distinct from the national program related to neutrino factory research. Firstly, we aim to examine various generic approaches to providing intense neutrino beams for high energy physics research. Secondly, we plan to make a site-specific study of building the first, low energy neutrino factory with an improved AGS as the injector on the present Brookhaven site. The goal of this program is to establish the feasibility of building a neutrino factory on the Brookhaven site and to establish the credibility of Brookhaven as a source of high energy neutrinos and detector competence for future long baseline neutrino oscillation experiments. This combination of a shorter term physics promise with a long-term accelerator development specifically aimed towards the exploitation of Brookhaven facilities and capabilities should strengthen our role in the overall muon collider and neutrino factory program.

APPROACH:

Our group is working in close concert with a large international collaboration on the possibility of building a neutrino factory. We have continued to work on the development of simulation tools for all aspects of the neutrino factory. We have explored how such a new facility could generate a more powerful and better defined neutrino beam than those that are currently available. The AGS or other proton source would generate muons, which would then be accelerated and stored in an elongated storage ring. Decays occurring in the straight sections of the ring would generate the neutrinos for the beam. The beam, so produced, could be directed to a detector located many thousands of km away and allow studies of neutrino oscillations in channels, and with precision, not currently possible. Designs of the muon capture, cooling, and acceleration needed for such a facility have been studied, including the special questions related to building the storage ring at an angle. Its potential to be upgraded for use as an injector into a muon collider has also been considered.

TECHNICAL PROGRESS AND RESULTS:

We began a formal study of the possibility of building a neutrino factory facility at BNL. Siting, civil engineering, geotechnical issues, such as radiation production and environmental impacts, and existing infrastructure questions have been considered. The Brookhaven proton accelerator, the AGS, is currently the most intense source at an energy suitable for driving a neutrino factory. We have explored upgrades of the AGS that would meet the full requirements for a neutrino factory, estimating the costs of such upgrades, and comparing these with proposals from other labs. The study has begun to identify areas of major uncertainty, crucial design issues, and topics requiring further theoretical or experimental R&D.

Detailed studies were made of the acceleration systems for the neutrino factory. The goal is to develop a technically feasible and economic scenario for accelerating the muon beam from 0.2 to 20-50 GeV/c. Design methods were perfected based on longitudinal phase space dynamics to ensure that the beam emittance fits in the rf bucket during acceleration. We began examining the relationship between accelerator parameters, such as frequency and gradient, and performance issues, such as emittance growth, dynamic losses and cost.

A basic linac design was constructed consisting of a phase rotation section for matching, a constant phase section to rapidly open up the bucket area, and a variable phase section to accelerate without emittance growth. It was found necessary to use a straight linac up to 3 GeV/c. An rf frequency optimization study examined the economic incentive to get to higher frequencies. It was found that 200 MHz was satisfactory from 0.2 to 0.7 GeV/c, while 400 MHz could be used from 0.7 to 3 GeV/c. Adding a third frequency at 800 MHz did not help.

The accelerator design for 3 to 20-50 GeV/c was based on racetrack shaped recirculating linear accelerators. A major design goal was to keep the beam matched with constant phase space area throughout the entire acceleration process. We considered the effects of additional design constraints, such as the number of turns, momentum acceptance of the arcs, and switchyard complexity. We found that it is advantageous to use a non-isochronous lattice, since that requires less energy acceptance in the arcs. The optimal solution found so far takes the beam from 3 to 12 GeV/c with four turns at 400 MHz and then from 12 to 50 GeV/c with 6 turns at 800 MHz. We also studied the possibility of using very large momentum acceptance FFAG lattices.

We began to study the question of the radiological consequences of building a neutrino factory at BNL. A comparison was made of the capabilities and limitations of transport simulation tools, such as MCNPX, GEANT and MARS. We found that tritium and Na22 were the main potential contaminants for the environment. We reviewed existing AGS neutrino target activation data for normalization of the studies. We then did MCNPX simulations of p, n and pions interacting with BNL soil and computed the tritium production as a function of energy. We studied the electromagnetic showers from muon decays in the arcs and straight sections. We used a specially modified version of GEANT to examine photoproduction of hadrons. We found that only a small amount of the shower penetrates the magnets. We found that direct interactions of neutrinos in the soil only produce a negligible amount of tritium.

SPECIFIC ACCOMPLISHMENTS:

J.S. Berg et al, Recirculating acceleration, in D. Cline (ed.), Physics Potential and Development of Muon Colliders and Neutrino Factories, AIP Conf. Proc. 542, 2000, p. 248-252.

J.S. Berg, Acceleration for a High energy Muon Collider, in B. King (ed.), Colliders and Collider Physics at the Highest Energies, AIP Conf. Proc. 530, 2000, p. 13-31.

LDRD FUNDING:

FY 2000	$194,812

Appendix A

2001 Project Summaries

Appendix A
BNL FY 2001 Projects

(01-07) Development of Superconducting Accelerator Magnets Capable of High dB/dt
A. Ghosh (FY 2001 Funding $145,000)

Extend the capabilities of superconducting magnets so that they can be ramped at much higher rates. This will require improvements in the NbTi superconductor as well as some magnet design. The ultimate goal is to design, fabricate, and test a proof-of-principle rapid ramping dipole magnet. This accomplishment could lead to the potential of constructing a superconducting synchrotron.

(01-11) Combination of Magnetic Fields and 20 keV Synchrotron X-rays to produce Microbeams for Cell Culture Experiments
L. Pena (FY 2001 Funding $11,396)

20 keV photons have sufficient linear energy transfer to deposit most of their energy in several millimeters of water consistent with available cell culture configurations, and use of a magnet will help the secondary emitted electrons to be transferred to a desired direction to maintain the sharpness of the microbeam with a calculation of the effort on the transport. Consequently, we will explore the development of a 20keV synchrotron X-ray beam combined with a 2 T magnetic field. This methodology will contribute to and extend the field of Medical Physics to enhance radiobiological research.

(01-12) Gene Expression Profiling of Methamphetamine-induced Toxicity in Neurons in Culture using DNA Microassays
M. Vazquez (FY 2001 Funding $99,800)

A new emphasis on the neuronal neurotoxicity is proposed which utilizes micro-array DNA chip technology to identify a specific set of genes in neuronal culture systems that respond to methaphetamine exposure. The goals are genome-wide expression analyses to identify gene-expression networks and toxicant-specific signatures that can be used to validate, 1) which set of genes is a key regulator of the toxic process, and 2) whether modulation of the gene is possible, and 3) if it will result in an amelioration of the neurotoxic process. In addition to providing state-of-the-art information on the application of DNA microarrays, high-resolution x-rays microscopy and image analysis technology for neurotoxicology studies, the project intends to catalyze the formation of several collaborations between BNL, SUNY Stony Brook, and LBNL using their unique scientific resources.

(01-13) "Functional Spectral Signature" (FSS) Method for Signal to Noise-Enhancement of Brain Patterns in PET Images
C. Felder (FY 2001 Funding $86,081)

Propose to develop and test an improved computer-based methodology to detect and quantitate faint differences in 3-dimensional functional brain patterns from groups of PET (Positron Emission Tomography) images and to enhance the signal-to-noise ratio by avoiding the blurring of images that is usually done to account for the anatomical and functional variability among subjects.

Appendix A
BNL FY 2001 Projects

(01-18) Exploration and Development of Ultrafast Single Short Detection Methods for Use with Pulse Radiolysis Experiments at LEAF
A. R. Cook (FY 2001 Funding $65,000)

A significant difficulty with radiation chemistry techniques can be the loss of sample and the buildup of radiation products following ionization. Propose to develop and construct a new experiment that will enable us to record transients in a single accelerator shot with a time resolution approaching 100 fs, three orders of magnitude better than current digitizers. Once constructed, this system will make possible many experiments, in particular observation of ultrafast electron transfer reactions with known energetics. Also plan to apply this new technique to the study of ultrafast electron transport in molecular wires, a topic of considerable current interest under the lab-wide nanotechnology initiative.

(01-19) New Program in Metal Nanocluster: Metal NanoClusters and Electron Transfer in One, Two, and Three Dimensions (NANO III)
C. Creutz (FY 2001 Funding $145,000)

Propose to make electron transfer measurements on an exceptional class of nano particles, Murray's Monolayer Protected Cluster Molecules (MPCs) in solution, at electrodes, and on surfaces to learn how electron-transfer rates change with these extreme changes in conditions. Will use nano clusters to characterize, model, and control electron transfer reactions in order to advance the design and construction of "molecularly wired," nanoscale devices.

(01-20) Molecular Wires for Energy Conversion and Nano-Electronics
J. R. Miller (FY 2001 Funding $50,000)

Use electron pulses from the Laser Electron Accelerator Facility (LEAF) to attach electrons or holes to "molecular wire" structures. Seek to demonstrate that spectroscopy on the electrons or holes in "wire" structures can give information about whether electrons (holes) are localized in the wires and do they become localized due to presence of added inert ions. Ultimately propose to construct computational models of the charge injection energetics.

(01-21) Nanoscale Catalysts: Preparation, Structure, and Reactivity (NANO II)
J. Hrbek (FY 2001 Funding $80,000)

Investigate and explore the use of dislocation arrays existing on the Au(111) surface (herringbone reconstruction) as a template for self-organized and tailored growth of metal and metal compound nanoclusters. Correlate the structure and morphology of nanoclusters with their chemical reactivity. Use single crystalline gold film grown on mica and vapor deposition to prepare the cluster arrays. Control the size and density of the nanoclusters by selection of deposition parameters. Characterize the model catalysts as to morphology, structure, and stability. Test reactivity of the catalysts for industrially relevant adsorbates using photoemission, IR, and high pressure kinetic measurements. This project will make an important contribution in the area of nanoscience in catalysis.

Appendix A
BNL FY 2001 Projects

(01-23) <u>Experimental and Theoretical Studies of the Formation of Titanium-Carbon Nanoclusters (NANO II)</u>
T. Sears (FY 2001 Funding $107,000)

This proposal describes experimental and theoretical investigations of the chemical and electronic properties of certain titanium metallo-carbohedrene (met-car) clusters and nanocrystals that have been found to be unusually stable. This stability is assumed to be related to a highly symmetric cage structure. Films deposited from plasmas are finding an increasing number of uses due to their hard and wear-resistant nature and this knowledge generated from this investigation will enhance their utility.

(01-24) <u>Development of a UV-Raman, Near-Field Scanning Optical Microscope for *in-situ* Studies of Chemical Intermediates on Metal Nanoparticles (NANO II)</u>
M. G. White (FY 2001 Funding $100,000)

The goal of this proposal is to develop UV-Raman, near-field optical scanning microscopy (NSOM) for *in situ* spectroscopic studies of catalytic reactions on small metal particles. Propose to couple the spatial resolution of NSOM with UV-Raman spectroscopy, which can provide a high degree of chemical information allowing for molecular identification and the determination of molecular orientation. The high sensitivity afforded by UV excitation counters the inherent low throughput of an NSOM device, making their combination a viable and potentially powerful tool for imaging adsorbed molecular species on isolated metal nanoparticles.

(01-26) <u>Nanoscience Interests (NANO II)</u>
J. Z. Larese (FY 2001 Funding $70,000)

Propose to use combined diffraction (neutrons, x-rays), electron microscopy and thermodynamic methods to understand and modify the growth characteristics of novel metal oxide particles or films, having the general chemical formula $R_xM_{1-x}O$ (where R=Mg, Zn, Cu and M=Ni, Cr, Mg, Zn, Ag, Au, Li ...). The primary aim would be to explore how changes in the composition and morphology of these materials affects the physical, chemical, mechanical, and magnetic properties. Want to be able to control and modify the synthetic process to produce pure and doped materials and, consequently, bypass the proprietary restrictions that usually accompany efforts of this type.

(01-28) <u>Development of New Techniques for Improvements in PET Imaging of Small Animals and Other Applications</u>
D. Schlyer (FY 2001 Funding $90,000)

The ultimate goal of this research is to build a detector that employs the latest technology in gamma ray detection to achieve the best possible energy and position resolution for Positron Emission Tomography (PET) imaging which can be used for a variety of applications, such as freely-moving small animal imaging, mammography, and many more. As a first step, a two-dimensional image will be obtained of a portion of the animal brain using standard imaging techniques employing commercially available scintillation crystals attached by optical fibers to photomultiplier tubes. As a second step, replace the photomultiplier tubes with avalanche photodiodes, along with their individual readout electronics, on each crystal. As the third step, explore replacing the original crystal arrays and APDs with two new arrays of crystals with smaller transverse dimensions and smaller area APDs and develop the microelectronics necessary for these arrays.

(01-30) Development of CZT Array Detector Technology for Synchrotron Radiation Applications
D. P. Siddons (FY 2001 Funding $107,000)

Many non-spectroscopic applications of synchrotron radiation are moving towards higher photon energies as a way to reduce sample absorption artifacts and to provide better bulk probes. Such applications would greatly benefit from the availability of a high-Z detector material and the technology for forming special-purpose arrays from this material. This proposal is to investigate the possibility of providing that technology within BNL. Propose to acquire high quality material from the various commercial vendors and assess its quality using both transport measurements and synchrotron radiation characterization methods, study the surface properties of the material with the goal of designing a reliable contact deposition technology, attempt to fabricate detector elements and element arrays using this technology, and to produce working detector systems.

(01-31) New Applications of Circular Polarized VUV-Light (NANO IV)
E. Voscovo (FY 2001 Funding $45,000)

Propose to develop the use of circular polarized VUV light produced at the U5UA beamline by means of a multiple-reflection polarizer. This addition will then enable the so-called complete spin-polarized photoemission experiment to be performed in which the polarization of both the incoming (photon) beam and the outgoing (electron) beam are under experimental control. This will have several applications in spectroscopic studies of solids in particular from magnetic materials.

(01-32) Soft X-Ray Magnetic Speckle (NANO IV)
C. Sanchez-Hanke (FY 2001 Funding $45,000)

Propose to develop a new magnetic imaging technique and the soft-x-ray version of the x-ray photon correlation spectroscopy (XPCS) using "magnetic speckle." Will exploit the strong domain orientation dependence of the resonant magnetic scattering amplitudes of 3d transition elements near the 2p absorption edges of these elements and the coherence soft-x-rays from X1 undulator to observe "magnetic speckle pattern." The objective is to develop a new magnetic domain imaging technique based on resonant x-ray scattering. The new capability could bring in a new user community into NSLS as well as benefit other core programs.

(01-35) Prototype Approaches for Infrared Nanospectroscopy
G. L. Carr (FY 2001 Funding $65,000)

Propose to test the limits of far-field infrared microscopy, investigate near-field methods, and design/develop a prototype near-field system for use with synchrotron radiation. Work will be conducted using the Northrop Grumman infrared microspectrometer system. The particular goals are to investigate the far-field limits for spatial resolution, including the use of high index materials such as ZnSe, KRS-5, and Ge; test the viability of image enhancement via point spread function deconvolution; develop plans for a scanning near-field probe system. This program is relevant to possible future light sources at the Laboratory such as FELs for infrared and other wavelength ranges.

(01-36) Pressure-Induced Protein Folding Monitored by Small Angle X-Ray Scattering and Fourier Transform Infrared Microspectroscopy
L. Miller (FY 2001 Funding $45,000)

The purpose of this proposal is to develop novel pressure-induced, time-resolved methods for studying the structure and dynamics of folding proteins monitored by synchrotron-based, small angle x-ray scattering (XAXS) and Fourier transform infrared micro-spectroscopy (FTIRMS). Will take advantage of the high brightness of synchrotron radiation, where x-ray and infrared beams can be focused through the small aperture of a diamond anvil pressure cell. Ultimately, this activity could lead to the development of a new method for obtaining protein structure analysis.

(01-38) Soft condensed Matter Probed by Low-Energy Resonant Scattering
W. Caliebe (FY 2001 Funding $45,000)

Propose to improve low-energy (1 keV to 3 keV) x-ray resonant scattering capability at X19A beamline at NSLS. An existing vacuum-compatible 2-circle diffractometer will be improved to have better sample manipulation and alignment.

(01-39) Femto-Second Transmission Electron Microscope Beam on Photocathode RF Gun
X. J. Wang (FY 2001 Funding $213,000)

Propose to design and experimentally demonstrate a femto-second transmission electron microscope based on the photocathode RF gun. The proposed transmission electron microscope will be capable of operating at energy from 300 keV to MeV for pico-second to femto-seconds time-resolved electron diffraction. The femto-second electron microscope based on a photocathode RF gun combined with other BNL facilities, such as NSLS, STEM, and Transmission electron microscope, will open new frontiers in many fields for time-resolved imaging.

(01-45) First-Principles Theory of the Magnetic and Electronic Properties of Nanostructures (NANO IV)
M. Weinert (FY 2001 Funding $90,000)

Propose to study the electronic and magnetic properties of nanostructure systems using first-principles approaches, and then to couple these results to simpler methods that can deal with larger length or time scales. Will use first-principles spin-density functional approaches to calculate the properties of nanoscale materials, including the determination of the geometry, magnetization and charge density profiles, and electronic states. This research is at the forefront of computational materials science, and will enrich the Laboratory's capabilities in modeling, computational science, and the interaction between theory and experiment.

(01-50) Cryo-EM for Solving Membrane Proteins
J. F. Hainfeld (FY 2001 Funding $118,000)

Purpose is to use cryo-electron microscopy to solve the human genome codes for membrane proteins by imaging 2-D membrane crystals at high resolution. Work will focus on adapting and using an existing electron microscope, cloning of membrane proteins to produce the amounts needed, preparation of 2-D membrane protein arrays, and data reduction to obtain structures.

(01-51) Human DNA Damage Responses: DNA-PK and p53
C. W. Anderson (FY 2001 Funding $168,000)

Propose is to identify genetic variations in the human non-homologous end-joining pathway (NHEJ) DNA repair system and to develop genetic systems to analyze these variations. Will also construct and characterize mutants that alter post-translational modification sites in the endogenous mouse p53 gene and characterize the biochemical and biological consequences of these mutants.

(01-52A) Molecular Mechanisms Underlying Structural Changes in the Adult Brain: A Genetic Analyses
J. J. Dunn (FY 2001 Funding $117,000)

The objective is to combine Serial Analysis of Gene Expression (SAGE), a powerful gene expression profiling method, and high-resolution 2-dimensional gel electrophoresis of proteins to investigate the mechanisms by which behavior through functional brain activation changes regional brain structure. Need to establish methodologies for mRNA and protein expression profiling from minute quantities of brain tissue from control animals (no exercise) and from exercised animals. Will identify genes that are activated in response to exercise and how these changes interact with the aging of the brain. In addition, this proposal will serve as the basis to develop methodologies to systematically assess the relationship between mRNA and protein expression levels.

(01-58A) Catalytic Microcombustion Systems
C. R. Krishna (FY 2001 Funding $96,000)

Will research all relevant processes and design and build a 100-watt microcombustor based on liquid fuel injection onto the system confining surfaces. Applications of this technology for microscale heat sources include: process heating (DNA replication on a chip), propulsion for micro robots and, microscale power generation via thermoelectric generation. Applications of mesoscale combustion technology includes heat sources for: manportable heating, heat actuated manportable cooling, manportable power generation via thermoelectric generation, and manportable water distillation.

Appendix A
BNL FY 2001 Projects

(01-59A) Power Quality and Reliability in Interconnected Microgrids
T. Butcher (FY 2001 Funding $75,000)

With strong growth expected in the use of distributed small electric power generation, there is great concern about the impacts of the quality of electric power and the reliability of supply. Will study both power quality, based on available microcogeneration equipment (fuel cells and microturbines), and reliability based on analysis of component failure rates. The end result will be a new capability and, in part, an extension of capabilities developed for nuclear reactors.

(01-62) Mapping Electron Densities in Prophyrin Radical Crystals Using the NSLS
K. M. Barkigia (FY 2001 Funding $30,000)

The goal of this research is to understand electronic structure in porphyrin radicals from single crystal X-ray diffraction data collected at the NSLS. Due to its inherent high precision, this work will unambiguously establish either localized or delocalized bond distance patterns in the porphyrin framework. Electron density studies of porphyrin radicals will provide simple answers to complex questions about structure and bonding that address the consequences of oxidation in vivo.

(01-67) High Sensitivity Mass Spectrometer
P. E. Vanier (FY 2001 Funding $121,000)

It is proposed to develop a new instrument which will improve on the state-of-the-art magnetic-sector mass spectrometer by at least an order of magnitude by making better use of the ions in the source. This advance will rely on the multiplexing of several narrow beams of ions defined by a coded array of slit apertures.

(01-78) Development and Application of Cavity Ringdown Spectroscopy to the Detection and Monitoring of Trace Chemical Species in the Atmosphere
A. J. Sedlacek (FY 2001 Funding $90,000)

It is proposed that a working proof-of-principle cavity ringdown (CRD) spectrometer system initially centered on mercury vapor detection be pursued. This system would serve as the principal unit from which issues associated with field use could be addressed as well as applicability towards other chemical species that possess near-UV/Visible absorption.

(01-79) Development of a High Field Magnet for Neutrino Storage Rings
R. Gupta (FY 2001 Funding $100,000)

Propose to develop and demonstrate a high field dipole magnet design in the range of 8-10 T, for a 20 GeV muon storage ring as a neutrino factory. The use of high field magnets would reduce the overall size of a storage ring and, in particular, high field magnets would permit placing the ring above the water table to minimize environmental impact.

Appendix A
BNL FY 2001 Projects

(01-82) DNA-Nano Wires that AutoConnect in 3 Dimensions (NANO III)
J. F. Hainfeld (FY 2001 Funding $60,000)

This study relates to nanocluster synthesis, charge conduction, quantum dots, nanocomputers, properties of nanomaterials, use of biological templates, and biotechnology. In particular, seek to reduce current lithographic 0.3 micron wires 150 times to 2 nm by placing gold quantum dots along a DNA template.

(01-85) Carbon Nanotube Chemical Probes for Biological Membrane Attachment Quantification (NANO III)
B. Panessa-Warren (FY 2001 Funding $49,800)

Carbon nanotubes will be covalently linked with specific compounds (lectins, nutritive molecules) to bind components of the exosporial membrane of Clostridial endospore pathogens, and these "loaded" nanotubes will be cultured with the activated endospores. Nanotubes will be produced with diameters of 1-25 nm diameter and many microns long, and thereby attached nanotubes should be readily visible by field emission scanning electron microscopy (FESEM). With this approach, the initial (reversible) and subsequent (irreversible) attachment structures of the spores can be mapped and the specific glycoprotein and/or exopolysaccharides identified.

(01-86) Self-Organized Nanoparticles for Probing Charge Transfer at Metallic/Organic Interfaces (NANO III)
M. Strongin (FY 2001 Funding $50,000)

The proposed work will use some of the unique properties of self-organized nanoparticle arrays to probe the transfer of charge at the interface between metals and organic materials. Specifically, will extend work on ultra-thin layers of metal deposited onto cryogenic substrates which were used many years ago to study the superconducting/insulator transition. Will be concerned with the effects of organic or biological molecules condensed onto the stable nanoparticle array. Both classical and quantum aspects of the arrays that will be studied.

(01-87) Charge Transfer on the Nano Scale: Theory (NANO III)
M. D. Newton (FY 2001 Funding $55,000)

Propose theoretical and computational work to provide compact interpretive, mechanistic models for nanoscale charge transfer phenomena, especially those of the type which will be targeted by the related experimental efforts. The primary thrust will be electronic structural computation and analysis, supplemented by suitable consideration of phonon and other inertial and diffusive features of charge transport systems.

(01-88) Charge Transport Through Dye-Sensitized Nanocrystalline Semiconductor Films (NANO III)
B. Brunschwig (FY 2001 Funding $55,000)

Propose to address what factors control the rate of charge transport in nanocrystalline systems and how does the rate depend on the nature of the particles and on their size and adsorbates and is particle-to-particle electron transfer inherently of low probability. Laser and pulse radiolysis electron injection will be used to initiate particle-to-particle charge transfer which will be followed using transient absorbance and photo-current measurements.

(01-91) Magnetic Nanodispersions (NANO IV)
L. H. Lewis (FY 2001 Funding $73,000)

It is proposed to investigate the magnetic properties as well-characterized thin-film magnetic nanodispersions with the ultimate goal of understanding the nature and extent of interparticulate magnetic interactions and how these interactions are mediated by the intervening matrix. The magnetic character will be investigated with complementary experimental techniques on a spectrum of length scales ranging from the atomic to the bulk. It is anticipated that knowledge obtained from these studies will not only enhance the body of basic knowledge of magnetism in composite materials but will also advance the nanoscale tailoring of such materials to specific parameters fostering novel and enhanced functionalities.

(01-93) High Resolution Magneto-Optical Study of Magnetic Nanostructures, Nanocomposite Functional and Superconducting Materials (NANO IV)
Q. Li (FY 2001 Funding $46,000)

Propose to utilize high resolution magneto-optical techniques with complementary transport, SQUID magnetization, and structural analysis to understand electromagnetic and structural properties of magnetic nanostructures, nanocomposite functional, and superconducting materials. Three classes of materials will be investigated: colossal magnetoresistive (CMR) oxides, magnetic nanostructure and multilayer heterostructures, and high temperature superconductors. Will emphasize the understanding of dynamic behavior of magnetic properties and its interaction with the nano-scale structural defects of these materials.

(01-94) Quantum Structure Fabrication and Characterization Using Advanced Transmission Electron Microscopy (NANO IV)
Y. Zhu (FY 2001 Funding $92,000)

Propose to fabricate and characterize samples with nanometerscale quantum structure such as quantum dots, wires, and helices for photonic and recording technology using our unique 300kV Transmission Electron Microscope (TEM) at BNL. The fabrication is based on nano-probe electron lithography. In-depth study of interphase interfaces using atomic imaging, electron induced x-ray spectroscopy, and electron energy-loss spectroscopy will shed light on the atomic structure, electronic structure, and magnetic coupling, hence the physical properties of the interfaces as well as of the materials.

(01-97) Size-Selected Quantum-Dots Under Controlled Environmental Conditions (NANO II)
D. Imre (FY 2001 Funding $90,000)

Femtosecond lasers will be used to probe the electronic dynamics of single-size quantum dots as small as 2nm or as large as 50nm in rare gas crystals. The dynamics of particle melting and crystallization will be investigated using novel pump-probe experiments at the NSLS. The effect of coating, encapsulation, and reactive treatments of single-size particle surface, on light emission, electrical conductivity and optical properties of single size nanocrystals will be explored.

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managed by Brookhaven Science Associates
for the U.S. Department of Energy

Memo

date: *June 1, 1999*

to: *Distribution*

from: *Peter Paul* Peter Paul

subject: *Laboratory Directed Research & Development Program (LDRD) Proposals*

This is to solicit proposals for the annual LDRD competition. The LDRD committee will meet in the last week of August to evaluate proposals for FY 2000 funding. Please submit proposals by August 15 through the respective Associate Laboratory Directors to the Director's office, using the attached proposal information and submission forms. To help you with the preparation of viable proposals, the BNL LDRD Manual and the DOE Directive DOE O 413.2, which defines the LDRD program, are also attached.

We have increased LDRD funds because we feel strongly that this program is essential for the long-term health and development of the Laboratory.

The evaluation Committee will, as in the past, consist of the Associate Laboratory Directors, augmented by selected distinguished scientists.

For FY 2001 there will be a change to the LDRD schedule. Proposals will be solicited on January 1, 2000, and are due March 1, 2000. Awards shall be made on April 1, 2000. This revision is to better facilitate the recruitment of post-doctorate students to support LDRD projects.

PP:KF:rp
Attachments

<u>Distribution:</u>

Department Chairpersons
V. Radeka
K. Fox

cc: Associate Laboratory Directors (w/o attachment)
Directorate (w/o attachment)

Exhibit B

The only official copy of this file is the one on-line in SBMS. Before using a printed copy, verify that it is the most current version by checking the document issue date on the BNL SBMS website.

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Issue Date: March 1999

Point of Contact: Laboratory Directed Research and Development Subject Matter Expert

Laboratory Directed Research and Development (LDRD) Program

I. Purpose

To encourage and support the development of new ideas that could lead to new programs, projects, and directions, the Laboratory will fund exploratory work by members of its staff.

II. General

The LDRD program focuses on early exploration and exploitation of creative and innovative concepts, which enhance the ability of the Laboratory to carry out its current and future mission objectives in line with the goals of the Department of Energy. This discretionary research and development tool is viewed as one important way of maintaining the scientific excellence of the Laboratory. It is a means to stimulate the scientific-technological community (foster new science and technology ideas), which is a factor in achieving and maintaining staff excellence, and is a means to address national needs within the overall mission of the DOE.

III. General Characteristics of the LDRD Program

Projects or studies that are appropriate candidates for the Laboratory Directed Research and Development Program (LDRD) are normally small, ranging from $50,000 to $200,000 per year, with a preference for smaller projects. They are generally funded for periods of two years with a possible continuation for a third year. Typically they include but are not limited to:

- Projects in the forefront areas of basic and applied science and technology for the primary purpose of enriching laboratory capabilities.
- Advanced study of new hypotheses, new concepts, or innovative approaches to scientific or technical problems.
- Experiments and analyses directed toward "proof of principle" or early determination of the utility of new scientific ideas.
- Conceptual and preliminary technical analysis of experimental facilities or devices.

IV. Procedures

Proposal preparation, submission, review and approval:

- Proposals will be solicited by January 1 for the following fiscal year. Awards will be made by April 1 on a competitive basis. Normally LDRD projects will start shortly after the beginning of the fiscal year.
- Applications should consist of a two- to three page proposal outlining the planned project. Applicants are encouraged to be brief but to provide sufficient information on the purpose of the project and the method of accomplishment. A copy of the Proposal Information Questionnaire **must** also be completed by the initiator and approved by the appropriate Department Administrator, Department Chairperson or Division Head. Completed applications are submitted to the Department Chairperson who forwards it to the Deputy Director for S&T who acts as the Chairperson of the LDRD Selection Committee.
- The LDRD Committee consists of the Deputy Director, the LDRD Scientific Director, all Associate Laboratory Directors, and two senior scientists chosen from the Brookhaven Council. The Committee reviews all proposals, obtains additional information deemed necessary, and selects the projects to be funded and the amount of each award.
- When an LDRD research project is authorized for funding, the principal investigator will be notified, as well as the cognizant Department Chairperson or Division Head. The Assistant Budget Office will establish a separate Laboratory overhead account to budget and collect the costs for the project.
- The total amount of funds to be made available for the program, and accordingly the number of projects supported, will vary from year to year, dependent to a large extent on the Laboratory's overall financial situation, and on the amount approved by DOE.

Reporting Requirements:

- In April of each year, the full LDRD Committee shall perform a formal mid-year review of all LDRD projects. This review will ascertain the progress and quality of the research performed.
- After the start of the project, interim annual status reports are required for each project and must be submitted by November 1 to the LDRD Scientific Director. These status reports should provide a brief summary (outlining purpose, approach, and status or progress of two pages or less) of the results of the LDRD project. Projects of more than one year should only summarize progress since the previous report. Additionally, the status report should also identify significant findings or accomplishments, papers, publications, patents, follow-on funding (includes funds requested or approved from other), support of post-docs or other students, presentations, and copyrights. For multi-year projects the goals for the following years should be updated in view of the previous year's experience.
- A written final report is required to be submitted within thirty days after the end of the project to the LDRD Scientific Director. The report should provide a summary of the results of the LDRD project as well as identify the significant findings, all papers, publications, patents, proposals, support of post-docs or other students, presentations, and copyrights that result from the study. If a proposal for new agency-funded research has been prepared, a copy should be enclosed with the report. If a proposal will be prepared, identify the funding agency and specific program and send a copy to the LDRD Scientific Director when it is submitted to the funding agency.

V. Restrictions

The purpose of the program is to develop new, fundable programs at Brookhaven. As such, the work proposed should be consistent with the missions of the Laboratory and the DOE and NRC. In this regard, the Laboratory's Institutional Plan and Agency program documents serve as guidance.

- Awards will not be made to substitute for, or increase funding for any tasks for which Congress or the DOE has established a specific limitation or for any specific tasks that are funded by DOE or other users of the laboratory.
- The exploratory study should not require the acquisition of permanent staff.
- It is expected that projects will be modest in size and limited to 3 years or less.
- The award will not fund activities that will require the addition of non-LDRD funds in order to reach a useful stage of completion.
- The LDRD study will not

1. fund construction line-item projects, in whole or in part,
2. fund construction design beyond the preliminary phase (e.g. conceptual design, Title I design work, or any similar or more advanced effort may not be supported),
3. Fund capital equipment expenditures. Any preliminary design work before conceptual design which is supported, must be directly associated with an LDRD project.

Exhibit C

BROOKHAVEN NATIONAL LABORATORY
PROPOSAL INFORMATION QUESTIONNAIRE
LABORATORY DIRECTED RESEARCH AND DEVELOPMENT PROGRAM

PRINCIPAL INVESTIGATOR ______________________ PHONE ______________

DEPARTMENT/DIVISION ______________________ DATE ______________

OTHER INVESTIGATORS ______________________

TITLE OF PROPOSAL ______________________________________

PROPOSAL TERM
From (month/year) ______________________ To (month/year) ______________

SUMMARY OF PROPOSAL Provide an abstract of the proposed project which clearly defines the central idea of the project scope, its purpose and what it hopes to accomplish. Also indicate how it meets the general characteristics of the LDRD Program. This should not exceed the space given below. Attach an extended proposal of no more then three (3) pages in length plus a milestone schedule.

Proposal

LDRD Milestone Schedule	
Date	Planned Accomplishments
Six Months	
1 year	
18 months	
2 years	
30 months	
3 years	

HUMAN SUBJECTS (Reference: DOE Order 1300.3)

Are human subjects involved from BNL or a collaborating institution?

If YES, attach copy of the current Institutional Review Board Approval and Informed Consent Form from BNL and/or collaborating institution. Y/N ________

VERTEBRATE ANIMALS

Are vertebrate animals involved? Y/N ________

If yes, has approval from BNL's Animal Care and Use Committee been obtained? Y/N ________

NEPA REVIEW

Are the activities proposed similar to those now carried out in the department/division which have been previously reviewed for potential environmental impacts and compliance with federal, state, local rules and regulations, and BNL's Environment, Safety, and Health Standards. (Therefore, if funded, proposed activities would require no additional environmental evaluation.) Y/N ________

If no, has a NEPA review been completed in accordance with the Subject Area National Environmental Policy Act (NEPA) and Cultural Resources Evaluation and the results documented? Y/N ________

(Note: if a NEPA review has not been completed, submit a copy of the work proposal to the BNL NEPA Coordinator for review. No work may commence until the review is completed and documented.)

ES&H CONSIDERATIONS

Does the proposal provide sufficient funding for appropriate decommissioning of the research space when the experiment is complete? Y/N ________

Is there an available waste disposal path for project wastes throughout the course of the experiment? Y/N ________

Is funding available to properly dispose of project wastes throughout the course of the experiment? Y/N ________

Can the proposed work be carried out within the existing safety envelope of the facility (Facility Use Agreement, Nuclear Facility Authorization Agreement, Accelerator Safety Envelope [ASE], etc.) in which it will be performed? Y/N ________

If not, what has to be done to prepare the facility to accept the work (modify the facility, revise the SAR/SAD, revise the Facility Use Agreement, etc.)and how will the modifications be funded? Y/N ________

FUNDING REQUESTED [ATTACH A DETAILED BUDGET BREAKDOWN]

[Break down the funding by fiscal year and by the broad categories of labor, materials and supplies, travel (foreign & domestic), services and subcontracts. LDRD funds cannot be used to purchase capital equipment. Indicate the intent to use collaborators and/or postdoctoral students, if applicable. Identify the various burdens applied, i.e., materials, organizational contracts. The Laboratory G&A should not be applied.]

POTENTIAL FUTURE FUNDING

Identify below the Agencies and the specific program/office which may be interested in supplying future funding. Give some indication of time frame.

Approvals

Department /Division Administrator ____________________

Department/Division Head ____________________

Cognizant Associate Director ____________________

BUDGET REQUEST BY FISCAL YEAR
(Note: Funding cannot exceed 3 years)

COST ELEMENT	FISCAL YEAR ____	FISCAL YEAR ____	FISCAL YEAR ____
Labor * Fringe Total Labor Organizational Burden @ ____ %			
Materials Supplies Travel Services Total MST Materials Burden @ ____%			
Sub-contracts Contracts Burden @ ____%			
Electric Power CCD Charge Other (specify)			
TOTAL PROJECT COST			
* Labor (indicate type of staff and level of effort)			
List all materials costing over $5000.			