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West Virginia

U.S. Department of Energy

Experimental Program to Stimulate Competitive Research

ABSTRACTS

Section II: Human Resource Development

Section III: Carbon-based Structural Materials Research Cluster

Section III: Data Parallel Algorithms for Scientific Computing

February 2, 1994

DISCLAIMER

Human Resource Development Plan and Activities for the West Virginia U.S. Department of Energy's EPSCoR Program

Abstract: Human Resource Development Plan

The objectives of the WV DOE/EPSCoR Human Resource Development (HRD) Plan are:

- to enhance junior faculty and student research in energy-related fields at the colleges and universities within the state through integrated, multi-institutional research clusters;
- to develop educational programs to transfer the knowledge and skills of those involved in the research clusters to others not directly involved;
- to foster interactions between researchers, educators at all levels, the US DOE, particularly the Morgantown Energy Technology Center, and industry;
- to support individual energy-related educational activities in grades K-12 to pilot more effective ways to teach science, engineering, and technological concepts to children in coordination with West Virginia's new science curriculum framework;
- to support educational activities targeted to groups traditionally underrepresented in the sciences, specifically females and minorities;
- to integrate all these activities with the development of the Rural Systemic Initiative and similar state-wide initiatives of the West Virginia Department of Education; and,
- through integration, build sufficient momentum and expertise to attract extramural funding for research and educational activities to sustain long-term continual improvements in the science, engineering, and technology human resources in West Virginia.

To meet the objectives, the plan includes K-12 enrichment activities, undergraduate research opportunities for students at the state's two Historically Black Colleges and Universities, graduate research through cluster assistantships and through a Traineeship Program targeted specifically to minorities, women and the disabled, and faculty development through participation in the research clusters.

Several project include both teacher enhancement activities and the direct involvement of school children. One of the K-12 enrichment activities will be active in a school with a large (33%) African American student body. And another targets a school with almost 90% of its children living in poverty. Both research clusters include women. One includes a minority faculty member. The Traineeship Program is targeted solely to underrepresented groups. And a mentoring program targets the states two Historically Black Colleges and Universities. Overall, 143 teachers and 865 students will be involved directly in the activities of the plan, while 32 more teachers and 2,420 students will become involved indirectly. Nineteen faculty members, 30 undergraduates, 11 graduate students, and 6 post doctoral fellows will also be involved in the overall program.

The plan is closely linked to the state's systemic reform initiatives in science and mathematics education. Key to the linkage is the role of Ms. Phyllis Barnhart, chief architect of the systemic initiative efforts, on the Human Resource Development Plan Advisory Committee. Each project supported under the K-12 enrichment activities also supports the systemic initiative goals.

Table of West Virginia U.S. DOE/EPSCoR Impacts
Human Resource Development Plan

Part One: Recipients of WV DOE/EPSCoR Human Resource Development Activities						
Institutions Involved	**K-12**		**College/University**			
A. Direct Involvement in WV DOE/EPSCoR	**Teachers**	**Students**	**Faculty**	**Under-grads**	**Graduate**	**Post-grads**
Programs for K-12						
1. (HRD-1-94) Hampshire County Board of Education, including Hampshire High and West Virginia Schools for the Deaf and Blind	6	220				
2. (HRD-2-94) Morgantown High School	1	50		2	1	
3. (HRD-3-94) Marshall University and six RESA II counties in surrounding area	12					
4. (HRD-4-94) Barnes Elementary School, Fairmont, Marion County	14	215				
5. (HRD-5-94) East Dale Elementary School, Fairmont, Marion County; West Virginia's First Science, Math and Technology Center (at East Dale)	90	180		10		
6. (HRD-6-94) Hugh Dingess Grade School, Harts, Logan County	10	200				
7. (HRD-7-94) Chemistry Workshop for High School Teachers (WVU)	10					
Programs for College/Universities						
1. (HRD-8-94) HBCU Mentoring Program			2	14		
Programs for Energy Research Personnel						
1. WVU Dept. of Chemistry, West Virginia Technological College, Marshall University (Carbon-based Materials Cluster)			10		6	6
2. WVU Dept. of Statistics and Computer Science, West Virginia Wesleyan College, Wheeling Jesuit College, Alderson Broaddus College (High Performance Computing Cluster)			7	4	4	

B. Indirect Recipients	K-12		College/University			
	Teachers	Students	Faculty	Uuder-grads	Graduate	Post-grads
1. (HRD-1-94) Hampshire County elementary and junior high schools	12 yr1 20 yr2	240 yr1 500 yr2				
2. (HRD-3-94) Marshall University and six RESA II counties in surrounding area		480				
3. (HRD-4-94) Barnes Elementary School, Fairmont, Marion County		200				
4. (HRD-5-94) East Dale Elementary School; West Virginia's First Science, Math and Technology Center		1,000				

Part Two: Providers of WV DOE/EPSCoR Human Resource Development Activities						
Institution Involved	K-12	Other	College/University			
	Teachers	Private Profes-sionals	Faculty	Uuder-grads	Graduates	Post-grads
1. (HRD-1-94) Hampshire County Board of Education	1	6	1			
2. (HRD-2-94) Morgantown High School	1	4	5		1	
3. (HRD-3-94) Marshall University			3		2	
4. (HRD-4-94) Barnes Elementary School	3	6	3			
5. (HRD-5-94) East Dale Elementary School	1	2	2			
6. (HRD-6-94) Hugh Dingess Grade School	1					
7. (HRD-9-94) WVU Dept. of Statistics and Computer Science			4			
8. (HRD-8-94) WVU Dept. of Chemistry			2			

West Virginia U.S. Department of Energy
Experimental Program to Stimulate Competitive Research

The Chemistry and Physics of Carbon-based Materials

Abstract: Chemistry and Physics of Carbon-Based Materials

The objective of this cluster is to develop a self-sustaining group of researchers in carbon-based materials research within the institutions of higher education in the State of West Virginia. The projects that are proposed focus on the research strengths of senior faculty with current work in this area and on the research strengths of junior faculty with developing interests in this area. The projects team senior and junior faculty so that a mentoring atmosphere is established. In some projects a senior faculty will take the lead and in others a junior faculty will take the lead. The cluster is arranged so that interactions among the team members are maximized. There is significant overlap of personnel among the projects and significant opportunities for postdocs and students to interact with all faculty. The concept of the team will be firmly established since the available equipment will be used in an inter-project mode, numerous samples will be studied in more than one project, many of the faculty have already established working teams and since numerous research discussions involving all cluster personnel will occur. The projects will involve analysis of cokes, graphites and other carbons in order to understand the properties that provide desirable structural characteristics including resistance to oxidation, levels of anisotropy and structural characteristics of the carbons themselves. This work fits within the interests of the Division of Materials Sciences of the USDOE Office of Basic Energy Sciences. This Division has interests in fundamental studies of materials including the surface chemistry and physics of carbon materials.

Project 1. Bulk and Surface Characterization of Carbon-Based Materials

Methods for the direct determination of the element composition in graphites and other carbon-based materials will be developed in this project. Work will focus on the refinement of previous developments in glow discharge mass spectrometry for the direct determination of trace elements. The limitations of the current methods when they are applied to carbon materials will be investigated and eliminated. In addition, sputtered neutral mass spectrometry will be developed into a reliable technique for the surface characterization of carbon materials. Therefore, bulk and surface characterization will be obtained. This work will involve Professor Fred King who is an expert in these techniques. He will interact extensively with Professor Paul Jagodzinski who has expertise in surface characterization of these materials using Raman spectroscopy. Some common samples will be used in both Projects 1 and 4 and the results will be combined to better understand the surface oxidation processes.

Project 2. Microprobe Studies of Novel Carbon Structures

Methods will be developed which will facilitate the study of the electronic properties of carbon materials of limited dimensionality (graphite, buckminsterfullerene and nanotubes). Attaching these materials to metal electrodes will permit surface studies using scanning tunnelling microscopy (STM). The methods of attachment will be developed within this project. Graphite will undergo site specific activation followed by gold deposition at these sites. These sites will then be selectively derivatized by attachment of molecules containing thiol groups (for example). The surface properties of the graphite will be investigated. Buckminsterfullerenes containing other molecules will be attached to electrode surfaces using clathrate structures. The electronic properties of these species on the surface will then be studied. The surfaces of nanotubes will be studied during the latter stages of the project. This work will be directed by Professor Michael Norton who will work closely with Professor Nar Dalal on the STM portion of the project. The results of the studies of the modified graphite in this project and the results of the

modeling work by Professor Cooper in Project 5 will be used to develop a more comprehensive understanding of the surface electronic properties of graphite.

Project 3. Investigation of the Corrosion Mechanism of Graphite Oxidation Products

Scanning tunnelling microscopy (STM) will be used to study the metal catalyzed oxidation of graphite surfaces. Previously developed techniques of forming well-defined metal clusters on surfaces will be utilized in order to examine gasification rates in a variety of technologically relevant atmospheric compositions and temperatures. In-air STM techniques will be used to form the metal clusters on surfaces which will then be subjected to various oxidizing conditions, and then characterized in a UHV equipped STM chamber. The effect of the size of the metal clusters on oxidation rates and whether metal clusters enhance the concentration of adsorbed oxygen at edge planes will be investigated. Studies to determine the effect of silicon coatings on graphite surfaces as a corrosion inhibition scheme will undertaken. This project will be directed by Professor Nar Dalal who will work in close association with Professor Michael Norton. This interaction will allow Professor Norton to have access to and learn UHV STM techniques. The results of this work will be important to the modeling performed by Professor Bernard Cooper in Project 5, a collaboration that already exists. The information will also be used by Professor Jagodzinski as he studies surface oxidation products in Project 4.

Project 4. Raman Spectroscopic Characterization of Graphite Oxidation Products

The oxidation characteristics of a suite of petrocoke and coal-based graphites will be studied using laser Raman spectroscopy. These studies will seek to identify the important molecular species and explain the mechanism of formation of oxidation products that give rise to recently observed new Raman signals. The graphites will be oxidized in controlled atmosphere conditions using times and temperatures determined in previous work. A database of information about the graphites (including source) will be developed and used in the analysis. Studies of diamond thin films produced in Project 1 will be initiated during the latter stages of this project. This project will be directed by Professor Paul Jagodzinski who will collaborate with Professor Fred King (Project 1) regarding the importance of trace element composition in the oxidation process. Professor Graham Rankin will collaborate in this work so that he can use his background in optical spectroscopy to develop expertise in the study of carbon materials using Raman spectroscopy. The information gained in Project 3 will also be important for the analysis portion of this project.

Project 5. Carbon-Based Materials: Computational Modeling

Full potential linear combination muffin-tin orbital (LMTO) methods will be used to model the corrosion susceptibility of carbon based materials. The work in this project will be based on recent success in modeling the effects of boron atom substitution, carbon vacancies, and iron atoms placed near a carbon surface on the surface electronic structure. In the current project the structural changes that are caused by point defects will be monitored through the associated relaxation processes. In conjunction with experimental work within the research cluster, 2-3 atom iron clusters will be placed at the carbon surface, and the effects of iron-surface interactions and iron-iron interactions will be monitored. This work will involve Professor Bernard Cooper, who will have extensive interactions with Professors Dalal and Norton (Project 3) and will interface with Professor Seehra (Project 7) and Professor Jagodzinski (Project 4).

Project 6. Control of Anisotropy in Coal Derived Graphites

The effects of preparation conditions on final product graphites will be monitored by analytical studies of intermediate materials (pitches and cokes) in the production of coal-based graphites. Two West Virginia coals, for which a reliable database of analytical analysis is available, will be used as starting materials. Parameters such as

reaction time, hydrogenation pressure and temperature and catalyst identity will be varied during the production of extracted pitch. Since the nature of the product graphite can be controlled by blending various pitch samples, a large suite of cokes will be produced and analyzed. The anisotropy of the cokes will be measured using polarized optical microscopy and the composition and structural characteristics of the precursors will be determined using the analytical expertise and instrumentation within the research cluster. This project will be directed by Professors John Zondlo and Alfred Stiller. They will serve as mentors for Professors Graham Rankin and Peter Stansberry who will broaden their current expertise and develop new expertise in the production and characterization of carbon materials. This project will rely on many of the other cluster investigators for analytical analysis.

Project 7. Determination of Structural Order in Carbons Using X-Ray Diffraction and Modeling

The structural parameters of disordered carbons will be investigated by obtaining x-ray diffraction (XRD) data and modeling this information with an available computer routine. The XRD of approximately 12 coal-based cokes and petrocokes will be collected before and after they are subjected to high temperature heat treatment. The analysis of this data will be aided by using computer codes that are based on One Layer and Two Layer Models for carbon materials. This work will permit insight into the correlation of coke properties with product graphite properties (previously obtained) and will allow the development of useful techniques for such analysis. There will be an attempt to use recent approaches to correlating XRD and Raman data to provide additional structural information. This project will be directed by Professor Mohindar Seehra who will work extensively with the researchers in Project 6. He will also work with Professor Jagodzinski (Project 4) in order to expand the latter's expertise in the use of Raman spectroscopy to study low frequency phonon modes in solids.

Relationship to WV US DOE/EPSCoR Human Resources Development Plan

The Human Resource Development Plan views the research clusters and the Traineeship Program as the key components for addressing the "human resource pipeline" at the graduate student level. Efforts are being made to diversify staffing of the clusters to allow for participation of underrepresented groups. Also, scientists in the Carbon-Based Structural Materials Research Cluster will participate in the High School Chemistry Teachers Workshop (HRD-8-94) to be developed by the Department of Chemistry.

Table of DOE/EPSCoR Program Impacts

Chemistry and Physics of Carbon-Based Structural Materials Research Cluster

Part One: Specific Projects within the Cluster and DOE Technical Program Area of Interest	
PROJECT TITLE	**DOE Technical Program Area, Contact Name, Phone, & Organization**
Bulk and Surface Characterization of Carbon-Based Materials	ER/BES/MS; R. Gottschall, (301) 903-3428; ER-131 (Dr. Gottschall is the contact for all the projects.)
Microprobe Studies of Novel Carbon Structures	
Investigations of the Corrosion Mechanisms of Carbon-Based Materials	
Raman Spectroscopic Characterization of Graphite Oxidation Products	
Carbon-Based Materials: Computational Modeling	
Control of Anisotropy in Coal Derived Graphites	
Determination of Structural Order in Carbons Using X-Ray Diffraction and Modeling	

Part Two: Information on the Institutions and Personnel Involved in the Cluster						
	Number of People Directly Involved					
	College/University				Pre-college	
Name of Institution	Faculty	Under-grads	Grads	Post-Grads	Teachers	Students
West Virginia University	8	0	5	6	0	0
Marshall University	2	2	2	0	0	0

Part Three: Equipment To Be Purchased					
EQUIPMENT ITEM	Proj. No.	Quantity	Unit Cost	DOE/ EPSCoR Funds	Matching Funds
Digital Oscilloscope	1	1	$20,000	$20,000	0
STM Update	2	1	$20,000	$20,000	0
AFM Head	3	1	$15,000	$15,000	0
Lexel Krypton Ion Laser Tube	4	1	$17,000	$17,000	0
Computer Workstation	5	1	$10,000	$10,000	0
High Temperature and Pressure Reactor	6	1	$15,000	$15,000	0
Computer Workstation	7	1	$10,000	$10,000	0

Part Four: Currently Funded or Pending Grants & Contracts Directly Related to the Research Cluster						
Funding Agency/Grant or Contract Title & Number	Principal Investigator Name/Institution	Contract/Grant Start Date	Contract/Grant End Date	$ Amount of Award	Funding Agency Contact Person Name	Funding Agency Contact Person Phone
Currently Funded:						
US DOE: Coal Based Nuclear Graphites for the New Production Gas Cooled Reactor (DE-FG02-91NP00159)	John Holmgren/WVU	3/1/90	2/28/94	$3,600,000	Sterling Franks	(202) 586-1279
Pending Funding:						
US DOE/PETC: Direct Determination of Trace Elements in Coal and Coal Products	Fred King/WVU	8/15/94	5/15/94	$197,315	Donna LeBetz	(412) 892-6206
US DOE/METC: Pollution Devices Based on Novel Forms of Carbon	J.W. Zondlo, et. al./WVU			$230,000		

West Virginia U.S. Department of Energy
Experimental Program to Stimulate Competitive Research
Data Parallel Algorithms for Scientific Computing

Abstract: Data Parallel Algorithms for Scientific Computing

In the proposed cluster, research by four WVU faculty and three state liberal arts college faculty in data parallel algorithms: (1) modeling self-organized critical systems by cellular automata, (2) multiprefix algorithms (extensions to the classical prefix algorithms) and fat-tree embeddings, (3) offline and online partitioning of data and computation, and (4) manipulating and rendering three dimensional objects.

The cluster furthers the state EPSCoR plan by building on existing strengths at WVU in parallel algorithms, using the CM-5 computer acquired in early 1993 as part of an NSF/EPSCoR program. Also, assisting liberal arts faculty currently enrolled in Ph.D. programs to continue in a research program after graduation and to collaborate with each other and WVU faculty.

Project 1: Extensions to Cellular Automata Model of Self-Organized Critical Systems

This project builds on work done by Per Bak, Michael Creutz, and others at Brookhaven National Laboratory. We propose to study variations on Per Bak, Creutz, et. al.'s transition functions (1) to find their mathematical properties and (2) to determine whether such functions better model physical systems. We also propose to study other open questions concerning such models. We will study our variations with the assistance of the CM-5 computer, acquired last year through the West Virginia NSF/EPSCoR program. This work, and the other projects in this cluster, complement the parallel algorithms research underway in the computational materials science cluster of the NSF/EPSCoR program.

Project 2: Data Parallel Algorithms Multiprefix and Fat-tree Embeddings

The prefix sum operator computes from vector A(1..N) to a new vector B(1..N) in which each B(I) is the sum of the I elements A(1), A(2), . . . , A(I). Efficient algorithms for prefix sum are well known. We have begun research on a multiprefix sum operator, in which each element of A is tagged as belonging to one of a small number of sets. B(I) is then the sum of all elements of A which have an index between 1 and I and which belong to the same set as A(I).

Many researchers have studied communications in parallel systems connected as meshes or hypercubes. The CM-5 computer available locally is organized as a fat-tree. We have begun studying efficient ways to map multidimensional meshes to m-ary fat trees.

Project 3: Effective Offline and Online Partitioning of Data and Computation

We propose to study variants of the k-server problem, with emphasis on variants involving some form of concurrency. Solutions and techniques for these online problems (i.e. problems whose inputs must be processed as they arrive, rather than in "batch" form) can be used to improve the performance of parallel and distributed computing systems. Particular areas of application include paging schemes,data placement and migration, and load balancing.

Project 4: Fast Algorithms and Software for Manipulating and Rendering Three Dimensional Objects

This project is related to work done by Chuck Hansen at Los Alamos National Laboratory. The primary goal of this proposal is to develop fast algorithms and software for manipulating and rendering three dimensional objects usable on parallel computers such as CM-5.. . Based on our experience with feature extraction on solid models we believe that topology of a solid object offers significant clues to partitioning an object. We are currently developing a parallel algorithm to perform set operations on 2D objects. This technique, is scalable to 3D operations as well. We are also planning to extend the use topological techniques for other applications such as rendering, interference checking, and geometric transformations (such as translation and rotation) on solid objects.

Relationship to the Human Resource Development Plan

The project leader, Dr. Frances VanScoy, herself a woman, will lead a mentoring effort for other women in the research cluster and for undergraduate students from the state's two Historically Black Colleges and Universities.

Table of DOE/EPSCoR Program Impacts

Data Parallel Algorithms for Scientific Computing

Part One: Specific Projects within the Cluster and DOE Technical Program Area of Interest	
PROJECT TITLE	DOE Technical Program Area, Contact Name, Phone, & Organization
Extensions to Cellular Automata Model of Self-Organized Critical Systems	Michael Creutz, Brookhaven National Laboratory
Data Parallel Algorithms Multiprefix and Fat-tree Embeddings	Dr. Charles Hansen, Los Alamos National Laboratory, P.O. Box 1663, M/S B287, Los Alamos, NM 87545
Effective Offline and Online Partitioning of Data and Computation	Tandy Warnow, Algorithms and Discrete Mathematics Department, Sandia National Laboratories, Albuquerque, NM. 505-845-7604, twarnow@cs.sandia.gov
Fast Algorithms and Software for Manipulating and Rendering Three Dimensional Objects	Dr. Charles Hansen, Los Alamos National Laboratory, P.O. Box 1663, M/S B 287, Los Alamos, NM 87545

Part Two: Information on the Institutions and Personnel Involved in the Cluster			
	Number of People Directly Involved		
Name of Institution	Faculty	Undergrad	Graduate
West Virginia University	4	1	4
Alderson Broaddus College	1	1	
West Virginia Wesleyan College	1	1	
Wheeling Jesuit College	1	1	

Part Three: Equipment - NONE TO BE PURCHASED UNDER THIS PROGRAM

Funding Agency/Grant, Contract Title	Principal Investigator	Contract/Grant		Amount of Award	Funding Agency Contact
		Start	End		
Currently Funded					
NSF/EPSCoR: Computational Materials Research Program (OSR-9255224); WV/EPSCoR Cost share	B. Cooper/ WVU	5/16/93	5/15/96	$2.1 million	R. Anderson, (703) 306-1683
DARPA: DARPA Initiative in Concurrent Engineering	R. Reddy/WVU	11/1/92	10/31/95	$9.7 million	L. Buchanan, (703) 691-2237
Pending Funding					
NSF: An Instrumentation Proposal for Computer Science	G. Trapp/WVU	7/1/94	6/30/96	n/a	n/a