DOE/CH/10482--1

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PLANNING OF A WEST VIRGINIA UNIVERSITY
RESEARCH CENTER IN THE BASIC MATERIALS SCIENCES

FINAL REPORT

SUBMITTED TO THE U.S. DEPARTMENT OF ENERGY
DOE FIELD OFFICE
ARGONNE IL
INSTRUMENT NUMBER: DE-FG02-91CH/0482

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March 1993

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I. INTRODUCTION

West Virginia University was provided a contract beginning in August 1991 to plan for the establishment of a research center in the basic materials sciences. The planning activity was to 1) identify the national need for a research Center which focuses on computational materials research, 2) identify the research projects which such a Center could conduct, 3) establish ties to industry so that the new Center can conduct research which can be applied to problems of commercial interest, 4) identify the personnel, equipment, and institutional needs to make the Center self-sustaining in terms of funding; and 5) plan and estimate the costs for facilities for the new Center.

In the proposal to the U.S. Department of Energy, WVU agreed to provide a report on the proposed programs for research for the new materials research Center, show how the Center is vital for national research and industrial needs, identify the computational and experimental equipment needed by the Center to fulfill its mission, list the facility requirements for the Center, and specify the way in which the Center will conduct interdisciplinary research in conjunction with national research laboratories and with industry.

This final report summarizes the results of this planning activity. Except for the planning for a new building to house the new Center (which has been indefinitely deferred), WVU has been very successful in completing all of the tasks identified in the original contract proposal. The research focus of the Center has been clearly identified, personnel have been put into place, research collaboration with industry has been arranged, interaction with DOE laboratories has been successful, and a three-year program of funding has been specified to support the research.

II. RESEARCH FOCUS OF CENTER

Through the planning grant activities, WVU was able to work with DOE technical managers, industry technical managers, and representatives of other agencies to identify a research focus for the new Center which was likely to grow in significance, had interest to industry and government, and was in an area in which WVU could develop expertise. The Computational Materials Research Center at West Virginia University uses the inherent advantages of parallel computers, an interdisciplinary group of theoretical and experimental physicists, computer scientists, and engineers to develop a new way of guiding industrial materials scientists and engineers in the development of better performing materials for applications to the energy, electronics, and transportation industries.

Materials scientists are increasingly recognizing that computational modeling can now realistically reduce the time and cost to develop new materials, or to solve perplexing materials performance problems by eliminating much of the trial and error used to identify materials for specific industrial applications.

In particular, the inherent computational advantages offered by parallel computers provide the potential to model accurately complications of materials systems including extended defects and dynamic effects, with a degree of realism previously unattainable. The materials research program underway at WVU seeks to link the three regimes of computational materials modeling, in work supported by materials synthesis and processing and experimental verification, into an integrated program and to do this on problems of direct industry interest. These three modeling regimes are atomistic modeling, microstructural modeling, and continuum modeling.

In order to conduct this research and to establish a program of national significance at West Virginia University, it is necessary to involve theoretical physicists, experimental physicists, material scientists, mechanical engineers, and computer scientists in a interdisciplinary program. A team of faculty has been organized at WVU from the departments of physics, statistics and computer science, and mechanical and aerospace engineering. In addition, faculty from the West Virginia Institute of Technology are now involved to bring more students and other West Virginia industry into the program. The following faculty are involved in the program:

B. R. Cooper, Project Director, WVU Physics

F. Van Scoy, Deputy Project Director, WVU Statistics and Computer Science

N. C. Giles, WVU Physics

L. Golubovic, WVU Physics

L. Halliburton, WVU Physics

B. S. Kang, WVU Mechanical and Aerospace Engineering

K. H. Means, WVU Mechanical Engineering

G. Mersten, WVIT Electrical Engineering

J. D. Mooney, WVU Statistics and Computer Science

T. H. Myers, WVU Physics

M. Seehra, WVU Physics

L. C. Wilson, WVU Physics

Research is being conducted on both structural and functional materials. A unifying feature of the phenomena to be predicted is their relationship to the interplay between electronic behavior and physical structure. Behavior at materials interfaces, including grain boundaries and/or the modification of materials functions through interfacing different

materials play a central role. An important part of the prediction and verification capability to be developed for structural materials behavior involves the ability to treat high-temperature behavior. Use of highly parallel computing is inherently advantageous for the modeling situations of interest, and the development and use of highly parallel computing will be emphasized. The computer scientists are supporting the work of the materials researchers by work in software quality. This work emphasizes raising the level of confidence in a given program and extending the range of usefulness for each program (by work in portability). In addition, the computer scientists are working with material researchers in developing new algorithms based on data structures other than matrices for representing materials structures. Their work is supporting that of the materials researchers by developing improved algorithms and higher quality software for modeling.

The research projects have been identified through the assistance of the Industrial Advisory Board. These are:

1. Modeling of metallic alloy systems for high-temperature structural applications. The objective of this work is the development of a computational materials modeling framework that includes atomistic, microstructural, and engineering continuum models. The work will include an effort to develop baseline understanding and computational methodology for the functioning of the protective oxide scale on superalloys used in high-temperature applications such as gas turbines. The work is aimed at treating several interconnected major aspects of deterioration of the protective functioning of the oxide scale; cracking and spallation due to coefficient of thermal expansion differences between the oxide scale and the underlying alloy, erosion of the protective oxide, and the resulting corrosion of the alloy. The work is leading to the development of capabilities for providing guidance to experimental work to control and improve CTE compatibility by the use of additive atomic species in nickel-based superalloys, as a function of nickel/chromium/aluminum composition. Work also includes an effort on analytical models of wear on erosion.

2. Atomistic origins of embrittlement effects with alloy. Research on this topic is being conducted on two aspects of alloy embrittlement, short range order effects and stress accelerated grain boundary oxygen (SAGBO) embrittlement. Development of short range order in nickel based alloys during long term elevated temperature service has been shown to result in mechanical instability and embrittlement. The computational models developed at WVU will test and find the scientific basis and empirical rules currently used to develop commercial alloys, and the empirical rules will be extended to consider the influence of various chemical species that are not now understood.

Numerous alloys and intermetallics are subjected to stress

accelerated grain boundary oxygen embrittlement (SAGBO) in which oxygen diffusion down grain boundaries results in intergranular failure and low ductility at temperature of about 538C or greater. Using WVU's molecular dynamics capability, the effects of additives based upon solid-state atomic size will be investigated as a means to solve this problem.

3. High temperature crack growth. This effort involves an investigation of crack growth behavior of nickel-based superalloys that are subjected to oxygen environmental attack at elevated temperatures. A combined micro and macro computational model is under development to correlate the microfracture process with the macro crack growth and evaluate related fracture parameters. This work will provide computational micro and macro analysis of environmental-assisted crack growth of nickel-based superalloys at elevated temperatures with experimental verification, investigate the influence of oxidation and grain boundary oxygen embrittlement on the particle coarsening of second-phase precipitation and the subsequent intergranular fracture, which cumulate in the macro crack growth of the alloy systems, and correlate the investigation with the atomistic modeling results.

4. Modeling of II-VI semiconductor superlattices for electrooptic applications. This work focuses on II-VI semiconductors which feature bandgap energies corresponding to wavelengths spanning the ultraviolet to the far infrared, thus giving the potential for light emitting diodes, lasers, detectors and other optoelectronic devices covering the entire spectrum. The research here consists of a coordinated, detailed theoretical and experimental investigation of superlattices in the Zn (Te, Se) materials system. These superlattices will be grown by molecular beam epitaxy (MBE). The synergism between detailed theoretical modeling and experimental investigations will result in progress in understanding the basic properties of II-VI superlattices. Band structure calculations based on techniques developed and demonstrated at WVU will be utilized for the inclusion of real interface effects such as relaxation and interdiffusion. The resultant model will allow prediction of the optoelectronic properties of the superlattices for a given configuration. In addition to determination of the dielectric properties, we are investigating the effects of defects and impurity atoms on the electrooptic properties. In parallel to the experimental growth studies, modeling of the growth dynamics will also be pursued using a combination of Monte Carlo and molecular dynamics methods. This will provide an understanding of defect formation during growth in order to control this parameter.

5. Highly parallel computer science research for materials

modeling. The computer scientists are performing work directed at improving the quality and performance of parallel software. Effective use of highly parallel computational facilities is vital for continued progress in materials modeling since suitable computational techniques using presently available hardware are not well developed. Thus, there is a need for more effective algorithms and for robust and adaptable software. Research by computer scientists includes work to develop improved parallel algorithms for selected materials problem domains by extending work in parallel algorithms and graph theory, and investigating techniques for improving the quality of software through more effective verification and increased portability.

III. INDUSTRIAL ADVISORY BOARD

Industry has been participating in the work of the Center by contributing in-kind and cash support, helping to identify research problems, providing feedback on research progress, and by serving as representatives on the industrial advisory board. The industrial advisory board is chaired by Mr. John deBarbadillo, Director of Research and Development Planning for INCO Alloys International, and including James C. Williams of GE Aircraft Engines, John Stringer of the Electric Power Research Institute, Scott Goodrich of Ravenswood Aluminum, Gernot H. Gessinger of Asea Brown Boveri-USA, Carl J. Johnson of II-VI Inc., Jesse Porre of Software Engineering Technology, Sokrates Pantelides of IBM, Tom Pressman of Strictly Business, Inc., and James Seydel of the Idaho National Engineering Laboratory. Two industrial advisory board meetings are held each year, the last being October 29 and 30 in Morgantown, West Virginia.

IV. INFORMATION DISSEMINATION

Information will flow between industry, government laboratories, and WVU through frequent work sessions. This format has already been established in developing the initial project on nickel/chromium alloys. The sessions involve industry describing pressing problems of interest and their thoughts on addressing these problems, and university personnel determining ways that computational approaches and experimental techniques could be used in attacking these problems.

Frequent sessions also are held with DOE staff and at government laboratories. WVU has been closely communicating with the DOE Office of Transportation Materials concerning work on lightweight materials for automotive applications. WVU has scoped out a research program with General Motors and Ravenswood Aluminum, and this work plan has been presented to technical managers at the Oak Ridge National Laboratory.

Information has also been widely disseminated though the annual Conference on Computational Research on Materials. The third conference is scheduled for May 2, 3, and 4 1993.

V. FUNDING

The planning grant itself allowed the Computational Materials Research Center to begin a demonstration project, in conjunction with the Idaho National Engineering Laboratory and INCO Alloys International to demonstrate the new approach under development. Additional funds were provided by EPRI (\$50,000), Asea Brown Boveri (\$65,000), and the West Virginia EPSCoR Program. However, the main source of funding for the program will be the National Science Foundations-EPSCoR Program. The State of West Virginia's EPSCoR Committee has recommended that this research activity be given three years of funding (beginning in April 1993) with \$600,000 in year 1, \$700,000 in year 2, and \$800,000 in year 3.

VI. COMPUTER FACILITIES

The new materials center now has a sophisticated parallel computer to conduct its research. This \$550,000 computer, a Thinking Machines CM-5 was installed in December 1992 to support the center and other activities in West Virginia. Additional funds for the purchase of this computer was provided by the National Research Center for Coal and Energy.

THIRD CONFERENCE ON COMPUTATIONAL RESEARCH ON MATERIALS

May 2-4, Morgantown, West Virginia

SECOND ANNOUNCEMENT

Chair: F.J. Calzonetti
West Virginia U.

Program Chairs:
B.R. Cooper
West Virginia U.

S.T. Pantelides
IBM Yorktown Hts.

Advisory Committee:
J. deBarbadillo
INCO Alloys

T. Gibbons
Asea Brown Boveri-USA

S. Goodrich
Ravenswood Aluminum

C. Johnson
II-VI Inc.

J. Poore
*U. of Tennessee-Software
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T. Pressman
Strictly Business Inc.

J. Seydel
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Laboratory*

J. Stringer
Electric Power Research Institute

J. Williams
GE Aircraft Engines

Arrangements for the Third Conference on Computational Research on Materials are well underway. The Conference will be held in Morgantown, West Virginia, on May 2, 3, and 4, 1993 at the Lakeview Resort and Conference Center. The 1991 and 1992 Conferences were quite successful and this year's program promises to be equally informative and stimulating.

The Third Conference on Computational Research on Materials will bring together leading researchers involved in computational materials research with technical managers and researchers from industry, government agencies, national laboratories and universities who are working to characterize, synthesize, process, and develop new materials systems. The objective of the Conference is to identify specific cases of the role of computational research in the national materials research agenda and to show how industry can use existing computational modeling capabilities and capabilities under development for such specific applications.

At the Conference, reports will be presented on the use of computational approaches to help design advanced materials more efficiently, at less cost, faster and with greater predictability of performance. This discussion will span the range from atomistic to mesoscopic to macroscopic modeling. This discussion will cover both structural and electronic materials systems. There will also be a discussion of the use of highly parallel processors for materials modeling problems and extended discussion of industrial research needs to provide better-performing materials more quickly, less expensively, and with greater predictability of performance.

Partial list of speakers and panelists: J. Bassani (U. of Pennsylvania), J. Broughton (Naval Research Lab.) J.W. Connolly (U. of Kentucky), B.R. Cooper (West Virginia U.), M. Daw (Sandia Nat. Lab.), P. Duxbury (Michigan State U.), P. Follansbee (Los Alamos National Lab.), E. Loh (Thinking Machines), A. Needleman (Brown U.), S.T. Pantelides (IBM), A.M. Stoneham (AEA Industrial Technology-Harwell), J. Taylor (Rutgers U.), F. Van Scoy (West Virginia U.) V. Viswanathan (EPRI), A. Voter (Los Alamos National Lab.).

The conference begins on Sunday evening with a reception and a keynote talk. The technical program consists of 30-minute talks and three panel discussions extending over all of Monday and Tuesday through lunch. At the end of the Monday sessions, there will be a 45-minute period of open discussion on the issues raised during the day. Conference participants will have the opportunity at that time to present one or two transparencies on relevant matters.

Thursday,
January 7, 1993

The Mountaineer SPIRIT

West Virginia University Faculty—Staff News

WVU purchases \$750,000 supercomputer

West Virginia University recently purchased an important new tool for solving scientific and engineering problems—a new generation, \$750,000 high performance massively parallel supercomputer. The computer system was installed last week at the West Virginia Network for Educational Telecomputing.

The Thinking Machines Corp. 16-node CM-5 computer is designed with a large number of processors so that complex scientific and engineering problems can be solved quickly and efficiently. Such computers are used in the physical sciences, health sciences, social sciences, humanities, mathematics and engineering disciplines.

WVU formed a research collaboration with Thinking Machines Corp., allowing the university to obtain the computer at less than the usual academic discount price. WVU and Thinking Machines will be working on joint research projects to demonstrate the use of the computer for a variety of important applications.

Funding for the purchase of the computer was made possible through the efforts of Sen. Robert C. Byrd, D-W.Va., who helped to obtain equipment funds for the National Research Center for Coal and Energy. Other funds were provided by NSF-EPSCoR program, the WVU Office of Academic Affairs and by a grant from the U.S. Department of Energy's Office of Basic Energy Sciences.

The computer will be used immediately by faculty and industry scientists and engineers who are working in the WVU Computational Materials Research Program.

Benedum Professor of Physics Bernard Cooper, director of the program, has been working with Associate Professor of Computer Science Frances Van Scoy in using parallel computers to assist INCO Alloys International and Asea Brown Boveri-U.S.A. identify ways to improve superalloys for use in gas turbines to produce electricity.

—Barbara Burke Ankrom

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