Laboratory Name: INEEL
B&R Code: KC020105

FWP and possible subtask under FWP:
"Center for Synthesis and Processing – Electroactive Polymers"

FWP Number: 3EB307

Program Scope:
This project is part of a multi-laboratory effort developed under the auspices of the Department of Energy (DOE) BES-Center of Excellence for the Synthesis and Processing of Advanced Materials. The objective of this research is to understand the mechanism of electronic transport through polymeric composite materials, which are formed in situ. The current emphasis is on understanding the controlling factors of electron anionic transport, such as microstructural, and physicochemical polymer ion properties by examining the electrophilic behavior of specified polymers. Additional effort in understanding synthesis and processing of platinum molecular wires is underway in collaboration with PNNL Center Member, and Montana State University.

Major Program Achievements (over duration of support):
Synthesis and characterization of platinum polymeric materials
Synthesis and characterization of mixed ligand platinum polymer materials
Synthesis and NMR characterization of a pure novel red phosphorescent compound

Program impact:
Certain heavy metal compounds can be caused to polymerize into linear chains, and these chains display metallic properties along one Cartesian axis but are non-metals along the other two. We have synthesized and characterized some of these polymeric materials that display one dimensional, truly metallic properties. These materials offer the opportunity to move electrical circuitry to the molecular level. This work continues using well-defined device properties for both macroscopic (bulk) and molecular level spatial scales. We plan to carry out the first investigations of their optical properties in the very near future.

Interactions:
Collaboration with Montana State University; one graduate student funded.
Professor Edwin H. Abbott, MSU; Professor Lee Spangler, MSU; Graduate Student Bernard Anderson, MSU.

Recognitions, Honors and Awards (at least partly attributable to support under this FWP or subtask):
None

Personnel Commitments for FY2002 to Nearest +/- 10%:
1.01 FTE (0.01 FTE Eric S. Peterson, INEEL; 1.0 FTE – Bernard Anderson, MSU).

Authorized Budget (BA) for FY00, FY01, FY02:
FY00 BA $16,000 FY01 BA $24,000 FY02 BA $25,000

Laboratory Name: INEEL
B&R Code: KC020603

FWP and possible subtask under FWP:
"Thermal Plasma Processing"

FWP Number: 3EE112

Program Scope:
This program is the experimental complement to the Thermal Plasma Processing Program. Both components are in their terminal year following the move of former PI J. Fincke to LANL. The intent of this last years' work is to optimize the harvest from previous years investments. Work will focus on comparison of measurements with simulations of plasma spray jet fluctuations and with modeled behavior of particles entrained in the jet (and the effects of turbulence and carrier gases thereon). It will also include investigation of the relationship between coating microstructure and plasma sprayed particle state as well as the preparation of manuscripts and the presentations of various papers.

Major Program Achievements (over duration of support):
The broad goal of this program has been to bring advances in diagnostics, data acquisition, and computation to bear in a unified experimental and theoretical research program to acquire a better fundamental understanding of the thermal plasma process. New experimental techniques which have been developed by the program include: (1) the simultaneous measurement of particle size, velocity, and temperature, (2) high resolution lineshape analysis of scattered laser light for direct measurement of plasma velocity, gas or heavy particle temperature, electron temperature, and electron density, (3) the development and validation of an enthalpy probe mass spectrometer system, and (4) the extension of various laser spectroscopic techniques such as Coherent Anti-Stokes Raman Spectroscopy and two-photon Laser Induced Fluorescence to the plasma environment. The diagnostic techniques developed under this project now represent the state of the art in thermal plasma processing.

Program impact:
Our strong commitment to collaborate with academic and industrial institutions has allowed the program to stay closely coupled to real problems and solutions in the thermal spray industry. Examples of technology transfer which are a direct result of research preformed under this program include: (1) collaboration with the National Center for Manufacturing and Ford Motor Co. to develop a miniature torch for spraying well defined coatings, (2) an industrial hardened particle temperature sensor, developed in a Cooperative Research and Development Agreement (CRADA) with TAFA Inc., the largest supplier of thermal spray equipment and consumables, and (3) recently a small company, Inflight, Ltd., has begun producing sensors and instrumentation for the thermal spray industry with much of the technology used in these products a direct result of research performed in this program. We currently have four externally funded CRADA's in place that are a direct result of our BES funded research efforts.

Interactions:
This program has enjoyed a continuing collaboration with the University of Minnesota, State University of New York at Stony Brook, University of Toronto and Boston University. In its final year, the program is partially supporting one Graduate Student at Boston University.

Recognitions, Honors and Awards (at least partly attributable to support under this FWP or subtask):

Accomplishments in advanced laser diagnostics have received international recognition as evidenced by invited plenary lectures at international plasma chemistry and thermal spray conferences and numerous invited papers.

Personnel Commitments for FY2002 to Nearest +/- 10%:
1.83 FTE (1.5 FTE INEEL Employees, 0.33 Graduate Student.)

Authorized Budget (BA) for FY00, FY01, FY02:
FY00 BA $467,000 FY01 BA $467,000 FY02 BA $467,000

Laboratory Name: INEEL
B&R Code: KC020603

FWP and possible subtask under FWP:
"Modeling of Thermal Plasma Processes"

FWP Number: 3EE114

Program Scope:
This program is the theoretical/modeling complement to the Thermal Plasma Processing Program. Both components are in their terminal year following the move of former PI J. Fincke to LANL. The intent of this last years' work is to optimize the harvest from previous years investments. Work will focus on simulations of plasma spray jet fluctuations, code and model development of the behavior of particles entrained in the jet (and the effects of turbulence and carrier gases thereon), documentation of recent LAVA code innovations, the preparation of manuscripts and the presentations of various papers.

Major Program Achievements (over duration of support):
The broad goal of this program has been to bring advances in diagnostics, data acquisition, and computation to bear in a unified experimental and theoretical research program to acquire a better fundamental understanding of the thermal plasma process. New computational capabilities which have been developed by the program include: (1) a numerical scheme for the fully implicit treatment of an arbitrary number of coupled nonequilibrium chemical reactions, (2) a formulation for multicomponent ambipolar diffusion in multitemperature thermal plasmas, and (3) a comprehensive particle model which includes multiple particle types, the calculation of internal temperature gradients, surface chemical reaction and internal diffusion of chemical species, the stochastic nature of the injection process, changing particle size due to vaporization, and the effect of vaporization on heat transfer and drag as well as plasma and non-continuum effects. The computational techniques developed under this project now represent the state of the art in thermal plasma processing.

Program impact:
Other investigators and research institutions have expressed considerable interest both in the theoretical formulations that have been developed and in the possibility of applying our computational model to their problems. For example, our multicomponent diffusion formulations are currently in use by Scientific Research Associates, Inc in their semiconductor processing simulations, at Lawrence Livermore National Laboratory in combustion simulations, at the Universite de Sherbrooke in plasma chemical reactor design. The broad impact of this research is indicated by the fact that these various organizations and proposed applications range all the way from basic research to industrial applications. Complete copies of the computational algorithm (the LAVA code) have been provided to 14 research groups worldwide and new requests are received regularly.

Interactions:
This program has enjoyed a continuing collaboration with the State University of New York at Stony Brook (SUNY-SB). In its final year, the program is partially supporting a graduate student and professor at SUNY-SB.

Recognitions, Honors and Awards (at least partly attributable to support under this FWP or subtask):
Recent recognition of results from this program include a best paper award at the 2000 International Thermal Spray Conference in Montreal, the cover photo for the December 2001 issue of the Journal of Thermal Spray Technology (JTST) and an invited paper in the March 2002 issue of JTST.

Personnel Commitments for FY2002 to Nearest +/- 10%:
1.49 FTE (0.7 FTE INEEL employee, 0.75 Graduate Student, 0.04 Professor).

Authorized Budget (BA) for FY00, FY01, FY02:

FY00 BA \$100,000	FY01 BA \$100,000	FY02 BA \$100,000

Laboratory Name: INEEL
B&R Code: KC020602

FWP and possible subtask under FWP:
Complex Intelligent Machines

FWP Number: 3EE113

Program Scope:
Experimental and modeling studies of heat and mass transfer in arc welding processes. Derivation of first principles model of droplet growth and detachment in gas metal arc welding. Experimental characterization of metal transfer dynamics in gas metal arc welding. Theoretical analysis of chaos in droplet transfer. Development of advanced sensing methods. Formulation of intelligent control methods, including learning and decision making algorithms.

Major Program Achievements (over duration of support):
Experimental characterization of spatial distribution of heat transfer from gas tungsten arcs to welding work-piece. Experimental measurements of droplet enthalpy in gas metal arc welding. Derived first principles model of droplet transfer in gas metal arc welding predicting chaotic dynamics. Experimental verification of chaotic dynamics in gas metal arc droplet transfer. Formulated fuzzy logic control algorithm without defuzzification. Derived equivalence of fuzzy logic control to classical control. Invented dry contact method for piezoelectric ultrasonic inspection of welds. Formulated method for sub-optimal discrete event decision making. Formulated new method for measuring fractal dimension of data sets.

Program Impact: Has enabled dry-contact ultrasonic inspection of welds on a pass-by-pass basis during welding for application to spent nuclear fuel canister seal welds (through DOE-EM funding). Has supported development of hybrid laser-gas metal arc welding process for industrial team (through DOE-OIT funding).

Interactions:
Massachusetts Institute of Technology; ORNL, Idaho State University; Utah State University; TACOM;
Institute of Production, Aalborg University, Denmark.

Recognitions, Honors and Awards (at least in some part attributable to support under this program):
H. B. Smartt - Editorial Board Member for the journal of Science and Technology of Welding and Joining, Key Reader for the AWS Welding Journal in automation, sensing, and control, member Technical Papers and Research and Development Committees of the American Welding Society, member AWS Presidential Task Group on NDE Certification, Spring 1997, thesis and dissertation committees at University of Idaho, Idaho State University, Massachusetts Institute of Technology, and University of Aalborg, awarded the A. F. Davis Silver Medal Award in the category of Machine Design by the American Welding Society in 1993, Co-Conference Chair: 4th International Conference on "Trends in Welding Research", Gatlinburg, TN, June, 1995, elected Fellow of the American Welding Society in 1997, Co-Conference Chair: 5th International Conference on "Trends in Welding Research", sponsored by ASM International, June 1998, received the AWS Adams Award in 1999 and presented the Adams Lecture at the AWS annual meeting in April 1999, Co-Conference Chair: 6th International Conference on "Trends in Welding Research", sponsored by ASM International, April 2002.

C. R. Tolle -- President of Rocky Mountain NASA Space Grant Consortium Fellows Association, Co-Deputy Director of the Rocky Mountain NASA Space Grant Consortium for INEEL, Assistant Adjunct Professor for the Department of Electrical and Computer Engineering, Utah State University, Awards Chair for the Eastern Idaho Section of IEEE, Vice-vice-chair of the Eastern Idaho Section of AWS and Past-President of the Wesley Foundation of Idaho State University, Senior member of the IEEE.

Personnel Commitments for FY2002 to Nearest +/- 10%:
1.35 FTE. [H. B. Smartt (30%), C. R. Tolle(30%), K. L. Miller(75%)]

Authorized Budget (BA) for FY00, FY01, FY2002:

FY00 BA $0	FY01 BA $200,000	FY02 BA $200,000

Laboratory Name: INEEL
B&R Code: KC020602

FWP and possible subtask under FWP:
"Microstructure Nondestructive Evaluation Using Imaging Laser Ultrasonics"

FWP Number: 3EE116

Program Scope: This research program is designed to probe materials microstructure as follows: I- Nonlocal Elastic Wave Imaging: uses elastic wave imaging and detailed theoretical modeling to determine the microstructural dependence of linear and nonlinear propagation that averages over many regions, such as grains. This work will be performed in collaboration with Professor Datta at the University of Colorado. Concurrent experimental imaging measurements utilizing the new elastic wave imaging approach developed at the INEEL are proposed to verify and corroborate the theoretical and experimental predictions of both programs. II- Local Elastic Wave Imaging: probes intragrain properties through a microscopic implementation of the imaging technique and evaluates it as a new microscopic measurement technique. III- Localized Source Elastic Wave Imaging: images and models the grain averaged elastic wave response produced by highly localized source mechanisms of varying kinds employing a "coupled mode" approach. Although many of these coupled mode methods are known and have been previously characterized, detailed research is needed to account for the material microstructure in the process. This work will be performed in collaboration with Dr. Martin Sablik at the Southwest Research Institute. Through collaborations, this INEEL research project will investigate not only unique experimental approaches to microstructure characterization but aid the development of the theoretical modeling to provide a basis for quantitative measurement. We believe that imaging will be an essential asset to obtaining this capability. And that this approach has a high potential for extending the ability of ultrasonic wave techniques to measure microstructural features relevant to quality control and lifetime issues in all structural materials.

Major Program Achievements (over duration of support):

(1) Performed the "first" experiments generating suboptical wavelength surface waves on material surfaces using optical means. [Phys. Rev. B 66, 153301-1 (2002).]
(2) Performed the "first" laser ultrasonic measurements of surface wave propagation through a single grain boundary (found enhanced nonlinearity) [Ultrasonics 40, 617-620 (2002).]
(3) Developed a GHz Acoustic Microscope for full-field imaging of acoustic wave motion on the nanosecond time and micron length scales. [2000 IEEE Ultrasonics Symposium Proceedings, Vol.1, 631-634 (2000).] [2002 IEEE Ultrasonics Symposium Proceedings, accepted for publication.]

Program impact: New information about elastic wave / microstructure interaction and new methodologies for obtaining that information have been determined. This new information provides a strong basis for mesoscopic scale testing in industrially important materials.

Interactions: This project included interactions and collaborations with on-going research at;
- University of Colorado (separately funded from DOE-BES), Professor Subhendu Datta, Chairman, Department of Mechanical Engineering and Professor Martin Dunn, Department of Mech. Eng.
- Southwest Research Institute (separately funded from DOE-BES), Dr. Martin Sablik, NDE Division.
- Agilent Technologies Inc., Palo Alto, CA, Dr. John Larsen, INEEL CRADA #00-CR-11 with Agilent Technologies Inc. "GHz Acoustic Microscope Measurements" FY2001- FY2003, $100.8K.
- University of Utah, Mathew Delong and Sergey Li, Department of Physics.
- Hokkaido University, Japan, Dr. Oliver Wright

Recognitions, Honors and Awards (at least partly attributable to support under this FWP or subtask): None (FY'02).

Personnel Commitments for FY2002 to Nearest +/- 10%: 1.25 FTE (INEEL employees).

Authorized Budget (BA) for FY00, FY01, FY02:

FY00 BA $300,000	FY01 BA $275,000	FY02 BA $300,000

Laboratory Name: INEEL
B&R Code: KC020202

FWP and possible subtask under FWP:
"Center for Synthesis and Processing – Nanomagnets"

FWP Number: 3E103

Program Scope:
This project is part of the Department of Energy (DOE) Office of Basic Energy Sciences Center of Excellence for the Synthesis and Processing of Advanced Materials. This five-year Center project titled, "Isolated and Collected Phenomena in Nanocomposite Magnets" involves a continuation of a previous five-year Center project titled, "Tailored Microstructures in Hard Magnets." The goal of this project is to team researchers from several DOE laboratories in a focused attack involving basic scientific studies of nanoscale nanocomposite magnets. Magnetic materials research underscores the mission of DOE since stronger magnets will allow the development of smaller, lighter, and more efficient electrical devices, thereby saving energy by increasing the efficiency of devices such as electrical motors.

Major Program Achievements (over duration of support):
This program has achieved the following awards:

"Great Advances in Scientific Discovery" nominated by The Science Coalition and presented to the 105th Congress for research on rare earth permanent magnets, 1998.

Top Performance Award**,** Lockheed Martin Idaho Technologies, 1998.

1997 R&D 100 Award for Development of "Nanocrystalline Composite Coercive Magnet Powder", 1997.

BES 1996 Materials Sciences Award for "Significant Implication For Department of Energy Related Technologies", 1996. It has resulted in 32 peer reviewed journal publications.

Program impact:
This project resulted in one DOE INEEL spin-off titled GA Powders. GA Powders was bought out by Magnequench International. The technology that has been developed is being produced resulting in worldwide magnet sales.

Interactions:
Collaboration with other DOE National Labs: specifically BNL, Ames, Oak Ridge, Los Alamos, and Argonne and Universities specifically Utah and Nebraska.

Recognitions, Honors and Awards (at least partly attributable to support under this FWP or subtask):
2002 TR100 Award for selection by MIT as one of the top 100 innovators under age 35 in the world.

Personnel Commitments for FY2002 to Nearest +/- 10%:
0.2 FTE (0.1 FTE for D. J. Branagan, 0.1 FTE for Brian Meacham – Post Doc at INEEL)

Authorized Budget (BA) for FY00, FY01, FY02:

FY00 BA $25,000	FY01 BA $25,000	FY02 BA $25,000

Laboratory Name: INEEL
B&R Code: KC020202

FWP and possible subtask under FWP:
"Structural and Electrostatic Effects in Self Assembled Nanostructural Growth"

FWP Number: 4B22-01

Program Scope:
A better understanding of the reconstruction of compound semiconductor surfaces is of considerable interest both in terms of increasing our fundamental knowledge and to facilitate our ability to synthesize these important materials. Work will examine the GaAs(100) surface and the vicinal GaAs(111)A/B surfaces focusing on the chemisoption related reconstructions on these surfaces. The hexagonal surfaces of wurtzite and zinc blende materials will also be studied in order to determine their detailed atomic structure. Emphasis will be placed on understanding how self-assembled nanostructures form on these surfaces. Factors influencing nanostructure growth such as strain, anti-site atomic positioning and localized electrostatic fields will be studied. Careful attention will be paid to the quantitative aspects of the surface analytical techniques used in this study.

Major Program Achievements (over duration of support):
- i.) Showed that anti-site atomic substitution, with concomitant electrostatic imbalances, contributed to nanostructure (island) formation on the B surface of GaAs(111) during homoepitaxy.
- ii.) Investigated competing aspects of electrostatic effects and strain in high aspect ratio nanostructures in potential spintronic materials.

Program impact:
Still in process. (Initial funding received Dec. 2001.)

Interactions:
Non-funded collaborations with Prof. C. J. Palmstrom, Univ. of Minnesota, and with Prof. G. J. Lapeyre, Montana State Univ.

Recognitions, Honors and Awards (at least partly attributable to support under this FWP or subtask):
None

Personnel Commitments for FY2002 to Nearest +/- 10%:
0.5 FTE (Helen H. Farrell)

Authorized Budget (BA) for FY00, FY01, FY02:

FY00 BA $0	FY01 BA $0	FY02 BA $150,000