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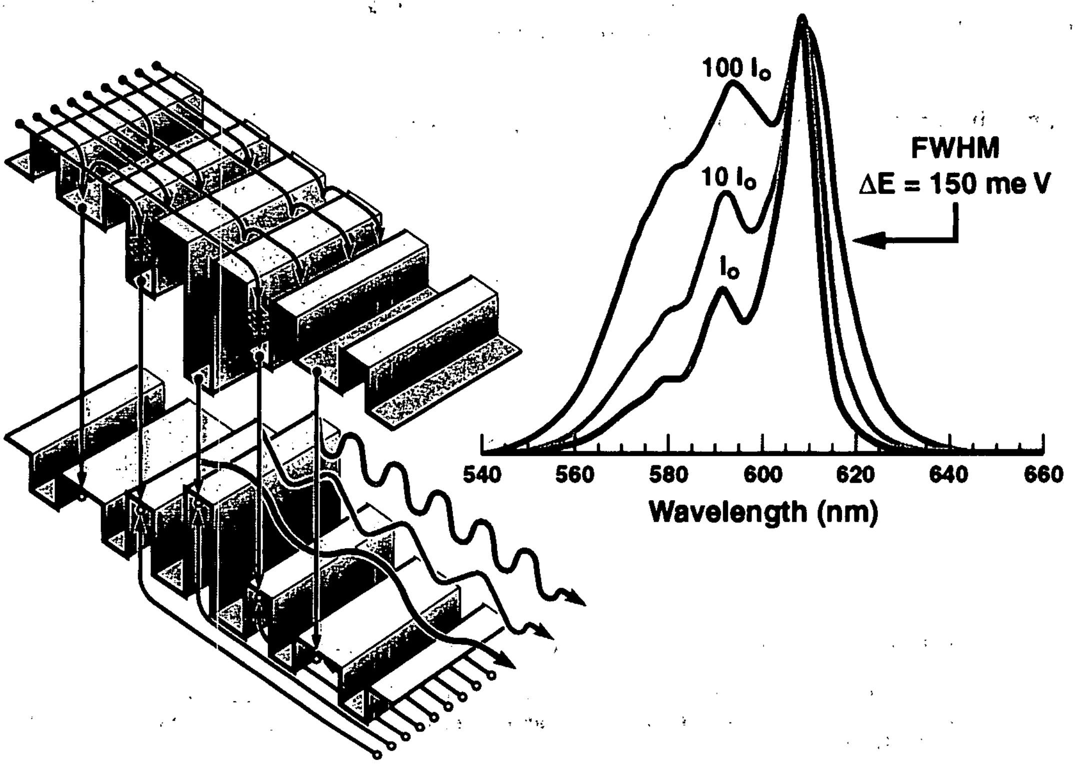

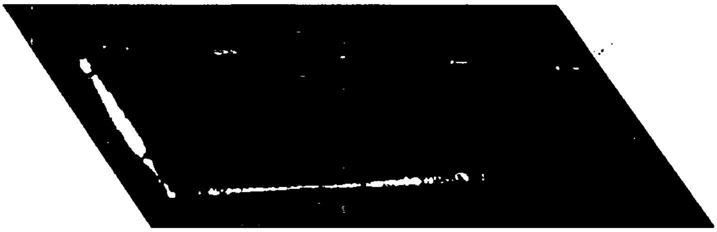

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Cover

A conceptual illustration of a new successful semiconductor device, a hybrid chirped/fractal quantum well design. The corrugated surface, corresponding to electronic quantum wells resulting from a layered semiconductor heterostructure, permits electrons streaming above the wells to selectively fall, via phonon coupling, into higher energy wells. The resultant recombination of electrons and holes give rise to photon emission at multiple wavelengths (see abstract #55 on page 35).

Figures and photograph courtesy of Paul L. Gourley, Sandia National Laboratories

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DOE/ER-0712

Advanced Energy Projects FY 1997 Research Summaries

September 1997

U.S. Department of Energy
Office of Energy Research
Office of Computational and
Technology Research
Advanced Energy Projects and
Technology Research Division
Germantown, MD 20874-1290

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APPENDICES

ADVANCED ENERGY PROJECTS

PROGRAM OVERVIEW

CHARTER

The mission of the Advanced Energy Projects (AEP) program is to explore the scientific feasibility of novel energy-related concepts that are high risk, in terms of scientific feasibility, yet have a realistic potential for a high technological payoff.

The concepts supported by the AEP are typically at an early stage of scientific development. They often arise from advances in basic research and are premature for consideration by applied research or technology development programs. Some are based on discoveries of new scientific phenomena or involve exploratory ideas that span multiple scientific and technical disciplines which do not fit into an existing DOE program area. In all cases, the objective is to support evaluation of the scientific or technical feasibility of the novel concepts involved. Following AEP support, it is expected that each concept will be sufficiently developed to attract further funding from other sources to realize its full potential. Projects that involve evolutionary research or technology development and demonstration are not supported by AEP. Furthermore, research projects more appropriate for another existing DOE research program are not encouraged.

SCOPE

The portfolio of projects is dynamic and reflects the Department's broad responsibility to support research and development for improving the Nation's energy posture and commercial competitiveness. Topical areas presently receiving support include:

- Alternative Energy Sources and Extraction Concepts
- Innovative Concepts for Energy Conversion and Storage
- Novel Approaches for Improving Energy Efficiency
- Biologically-Based Energy Concepts
- Advanced Materials for Energy Technology
- Novel Materials and Processes for Waste Elimination
- New Energy-Related Phenomena

Within these topical areas, AEP supports a range of research disciplines including physics, chemistry, materials science, geoscience, engineering, biotechnology and interdisciplinary projects.

FUNDING

Projects are supported for a specified period of time, which typically does not exceed three years. In Fiscal Year 1997, the average annual funding level for an AEP project was $250,000 and the average funding period was about three years.

SUBMISSION GUIDELINES

Projects supported by AEP arise from unsolicited ideas submitted by researchers. Unsolicited proposals can be submitted by universities, industrial organizations, non-profit research institutions, or private individuals. AEP also considers ideas or concepts submitted by researchers at national laboratories.

PREPROPOSALS

Before a formal proposal is prepared, the proposer should submit a summary (3-5 pages) of the proposed work to AEP for consideration. The summary should outline the scientific concept. It should contain enough information to enable an informed decision as to whether the proposed work would be programmatically suited to the charter of the Advanced Energy Projects program. It should include concise descriptions of the proposed work and its potential benefit to energy science and technology. The summary should also contain estimates of the funding period and of the annual funding level. If possible, some discussion of anticipated follow-on funding scenarios should be provided.

PROPOSALS

After an AEP programmatic interest has been established, a proposal must be submitted consistent with the guidelines specified in the document, DOE/ER-0249, "Application Guide for the Office of Energy Research Financial Assistance Program - 10 CFR Part 605, Issuance No. 3.1" (http://www.er.doe.gov/production/grants/guide.html). In addition to these requirements, a 200-300 word abstract describing the project should be included in the proposal.

PROPOSAL EVALUATION

Awards are based on the results of an evaluation process that includes independent reviews by external scientific and technical experts. The review process is the same for all submissions. Regardless of the outcome of the evaluation, proposers receive copies of reviewers' reports.

Questions asked of the reviewers depend on the subject of the proposal, but usually include the following:

1. What is the scientific and technical merit of the proposed effort?
2. Is the proposed effort innovative? How does it compare with other work? Is the proposed effort an extension or continuation of an earlier discovery or breakthrough, or is it, in itself, novel or unique?
3. Are there basic flaws or major shortcomings in the scientific or technical arguments underlying the concept?
4. Are the technological and/or material requirements associated with the proposed concept within present or near term capabilities?
5. Is there anything about the concept that makes its economics manifestly untenable, even under reasonably optimistic assumptions?
6. Is the anticipated benefit to the public high enough to warrant the Department of Energy's involvement in the R&D effort?
7. How well does the proposed research match the AEP charter?

CONTACTS IN AEP

- Dr. Walter M. Polansky, Director
- Mr. David E. Koegel*
- Ms. Sue Ellen Stottlemyer

Advanced Energy Projects and Technology
Research Division
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Phone: 301/903-5995
Fax: 301/903-6067 (no more than 10 pages; also see Appendix D)

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*On detail from the Office of Planning and Analysis, Energy Research

This book was compiled by Sue Ellen Stottlemyer.

This document also appears on the World Wide Web at http://www.er.doe.gov/production/octr/aep/aephome.html

The homepage for the Advanced Energy Projects and Technology Research Division appears at: http://www.er.doe.gov/production/octr/aeptr/aeptr_pr.html

SUMMARIES OF PROJECTS ACTIVE IN FY 1997

GRANT AND LABORATORY PROGRAMS

There were 65 projects in the Advanced Energy Projects research portfolio during Fiscal Year 1997 (October 1, 1996 - September 30, 1997). Eighteen projects were initiated during that fiscal year. See Appendix B for FY 1997 budget information. Further information on a specific project may be obtained by contacting the principal investigator. **Note - To accommodate the limitations of the World Wide Web format, subscripts and superscripts are suppressed in the project summaries below.**

American University
Washington, DC 20016-8058

1. Accelerated Beta Decay for Disposal of Fission Fragment Wastes

Howard Reiss
Department of Physics
202/885-2749

Funding Profile
Date Started: June 15, 1996
Anticipated Duration: 2 Years

FY 96 - $123,000
FY 97 - $ 99,000

This project is focused on the development of a detailed theory for the acceleration of the so-called "forbidden" (actually just strongly inhibited) beta decays exhibited by fission fragment wastes. These wastes constitute the bulk of the radioactivity of nuclear reactor waste products for about the first thousand years after removal from a reactor, so a significant acceleration of the decay rate by a low cost method would present major benefits. The acceleration scheme depends upon the observation that each degree of forbiddenness in beta decay causes an extension of half life by a factor of about 10(4), and arises from a violation of quantum selection rules in the decay process. These selection rules involve only angular momentum and intrinsic parity, and it is proposed to supply these by coupling of a low frequency electromagnetic field to the nucleus. No energy needs to be contributed by the field - the fission fragment already possesses the necessary energy, which it would emit relatively quickly were it able to satisfy the quantum selection rules. Under normal circumstances, it is not possible to couple effectively a long-wavelength field to the nucleus because of the severe mismatch in sizes. It can be shown, however, that a very intense field provides qualitatively different coupling than is apparent from the perturbative (weak-field) coupling. Specifically, perturbation theory predicts that the coupling depends on the ratio of the field nucleus interaction to a characteristic nuclear energy. It is impossible to achieve a significant value for this ratio with low frequency fields. By contrast, intense-field theory shows that the coupling depends on the ratio of the field-nucleus interaction energy to $\hbar\omega$, where ω is the circular frequency of the external field. This last energy is far smaller than a nuclear energy, and a practicable value of the coupling ratio can be achieved.

Ames Laboratory
Iowa State University
Ames, IA 50011-3020

2. Magnetic Refrigeration for Sub-Room Temperature Cooling

Karl A. Gschneidner, Jr.
Metallurgy and Ceramics Division
515/294-7931

Funding Profile
Date Started: April 15, 1994
Anticipated Duration: 3 Years (Project Completed)

FY 94 - $360,000
FY 95 - $304,000
FY 96 - $310,000

The design of a new type of near-room temperature magnetic refrigerator and the demonstration of its technical feasibility as an alternative refrigeration technology for energy-intensive industrial and commercial refrigeration systems is under development. Large-scale (>30 kW) chlorofluorocarbon (CFC) vapor cycle refrigeration units in commercial facilities, such as deep-freezers in meat packing plants and display case chillers in supermarkets, represent a significant portion of the total U.S. electrical energy demand. The efficiency of existing refrigerators is considerably less than that of the ideal Carnot efficiency because of intrinsic limitations of the currently used vapor cycle process, especially in the compression and Joule-Thomson expansion parts of the cycle. In contrast, the magnetic refrigeration cycle has a very high intrinsic efficiency; the efficiency appears to be limited by factors amenable to control, such as non-ideal materials properties, parasitic heat transfer, and flow losses. Replacement of vapor cycle refrigerators with magnetic refrigerators offers a significant potential energy savings. In addition, magnetic refrigerators do not require any ozone-damaging CFCs or other volatile fluids that have a significant greenhouse effect, so their widespread use would reduce potential environmental hazards. The elimination of CFCs is also in compliance with federally mandated programs to reduce the risk to the ozone layer. There are two major aspects of this project. The first is a materials development task, which will be carried out by the Ames Laboratory in Ames, Iowa. The second task involves the engineering aspects of designing, constructing, and demonstrating a sub-room temperature active magnetic regenerator magnetic refrigerator, which will be carried out at the Technology Center of the Astronautics Corporation of America, in Madison, Wisconsin.

Ames Laboratory
Iowa State University
Ames, IA 50011-3020

3. Composite Magnetostrictive Materials for Advanced Automotive Magnetomechanical Sensors

David C. Jiles
Metallurgy and Ceramics Division
515/294-9685

Funding Profile
Date Started: September 15, 1996
Anticipated Duration: 3 Years

FY 96 - $101,000
FY 97 - $449,000
FY 98 - $270,000

There is a well established need for torque sensors for a variety of applications in automobiles. Such sensors can be used for electronic control of the vehicle by monitoring steering and drive train torques. In this project, new highly magnetostrictive materials are being investigated for use in advanced steering systems. Such sensors will eliminate the need for maintaining a pressurized hydraulic power steering system and will improve fuel efficiency by 5%. These sensors will need to meet stringent specifications such as the ability to operate over a range of temperatures between minus 40° C and plus 85° C, be able to survive unexpected mechanical shocks of up to 500 N and operate under continual vibrational forces of 150 N. In addition, the sensors must be able to sustain overload torques of 135 N.m without malfunctioning or significantly changing sensitivity over the normal operating range of +/- 10 N.m. Analysis of the relationship between the magnetomechanical effect (the change in magnetization with stress) and the magnetostriction (particularly the rate of change of strain with magnetic field) has shown that highly magnetostrictive materials with low anisotropy, and hence high permeability, form the most promising class of materials from which to develop such high performance sensors. This project is therefore investigating the fabrication of composite materials consisting of the highly magnetostrictive material Terfenol-D in a high-strength matrix material, in order to meet the performance specifications for these torque sensors.

Ames Laboratory
Iowa State University
Ames, IA 50011-3020

4. Next Generation High-Temperature Structural Materials for Heat Exchangers and Heating Elements

Mufit Akinc
515/294-0744

Funding Profile
Date Started: January 15, 1997
Anticipated Duration: 3 Years

FY 97 - $294,000
FY 98 - $297,000
FY 99 - $305,000

The project is centered on the development of a new generation of electrical furnace heating elements and heat exchangers. Existing materials for heat exchangers and heating elements are limited by their mechanical and/or oxidative stability at high temperatures. MoSi(2) is limited by its low creep strength above 1000° C whereas other metallic or intermetallic materials are limited to about 1000° C. Increasing the temperature capability of existing heat exchangers and heating elements by several hundred degrees and/or providing alternative furnace designs will provide significant energy efficiencies as well as ecological benefits. Recent work in our laboratory shows that boron doped Mo(5)Si(3) exhibits outstanding oxidative stability in addition to its excellent high temperature creep strength and high melting point. However, a number of scientific and technical issues remain to be elucidated. An integrated multi-disciplinary approach to synthesis and processing, microstructural, thermomechanical and electrical investigation of select compositions around Mo(5)Si(3)B is being pursued. The investigation will focus on establishing the fundamental relationship between composition, microstructure, and physical properties of B-doped Mo(5)Si(3). In particular, select compositions will be synthesized and sintered to produce dense parts. A number of compositions will be studied for their stability in air and in corrosive atmospheres up to 1500° C. Thermomechanical properties of successful compositions will be investigated as a function of temperature and will be related to their microstructure. Thermoelectric properties such as thermal and electrical conductivity will be determined at temperatures up to 1500° C and above. Optimum compositions will be determined and process scale-up will be considered for heating element and heat exchanger applications.

Argonne National Laboratory
9700 South Cass Avenue
Argonne, IL 60439-4831

5. Iron-Sulfur Chemistry in Petroleum Production

Mark R. Antonio
Chemistry Division
630/252-9267

Funding Profile
Date Started: December 15, 1995
Anticipated Duration: 3 Years

FY 96 - $302,000
FY 97 - $298,000
FY 98 - $300,000

It is our concept that fundamental knowledge about the subsurface reservoir chemistry of iron and sulfur can be exploited to improve U.S. oil production from souring reservoirs. To realize this concept, this project focuses on three scientific-technological issues concerning biotic and abiotic ferruginous sulfides, Fe-S, which plague secondary (i.e., waterflood) oil recovery operations. These microbiologically-mediated and chemically-produced sulfides contribute to well fouling, a problem that can completely ruin the production of a reservoir. The first program thrust area concerns studies of the origins, and the interrelationships of these sulfides under different conditions of temperature, pH, salinity, pressure, concentrations of iron and hydrogen sulfide, in combination with the presence of sulfate reducing bacteria. To complement these studies, the second thrust area involves the characterization of the Fe-S species by use of a suite of spectroscopic and analytical techniques. The fundamental understanding of iron-sulfur chemistry to be gained from this integrated research plan will provide otherwise unavailable insights about the speciation of iron in produced waters, and essential information about well fouling in subsurface oil reservoir formations. The third thrust area concerns the development of Mössbauer spectroscopy for field measurement and identification of iron-bearing solids at the drill site. We plan to design a rugged, transportable Mössbauer instrument to acquire data that will provide definitive information about the iron speciation in the downhole environment. A comprehensive knowledge of the exact chemical and physical state of iron in production zones and waters should enable the selection of appropriate and phase specific chemical treatment programs to effectively offset declines and increase oil production in U.S. fields. The use of such a field capability during production operations will facilitate the controlled exploitation of our national oil reserves. The success of this project could lead to a significant breakthrough in oil field technology that will result in enhanced oil recoveries at reduced cost.

Argonne National Laboratory
9700 South Cass Avenue
Argonne, IL 60439

6. Tritiated Porous Silicon: A Stand-Alone Power Source

Carl E. Johnson
630/252-7533

Funding Profile
Date Started: November 15, 1996
Anticipated Duration: 3 Years

FY 97 - $250,000
FY 98 - $260,000
FY 99 - $270,000

Tritiated porous silicon could form the basis for a new class of stand-alone power sources that are rugged and portable and have high reliability over a very long period (>10 yr.). The tritium is covalently bonded to the silicon and, thus, cannot escape as a gas into the environment. This material would be able to provide the relatively low-level power requirement of many types of highly integrated devices in optoelectronics and sensor technology. The proposed research involves three tasks: 1) demonstrate the synthesis of tritiated porous silicon; 2) model the synthesis process; and 3) assess the optical activity of this novel material. The objective of this project is to attain proof-of-concept and lay the foundation for development of a commercial device. The data base resulting from the proposed work would provide a firm foundation for future engineering design efforts aimed at device development for specific applications.

Argonne National Laboratory
9700 South Cass Avenue
Argonne, IL 60439

7. Novel Biomimetic TiO(2) Photocatalysts for Removal of Selective Heavy Metals

Natalia K. Meshkov
630/252-5234

Funding Profile
Date Started: November 15, 1996
Anticipated Duration: 3 Years

FY 97 - $345,000
FY 98 - $325,000
FY 99 - $305,000

This project expands upon our recent invention of a photocatalyst capable of complete removal of highly toxic lead ions from aqueous solutions and their reduction to metallic form. Multi functional ligands were used to form charge-transfer complexes with nanosized TiO(2) particles and to bridge the colloid particle surface to the heavy-metal ions. This approach sequesters metal ions and enhances the reducing properties of TiO(2), making the photocatalytic process accessible to a whole new class of heavy-metal ions with relatively negative reduction potentials. The optical absorption of surface-modified TiO(2) is shifted from ultraviolet into the visible region, enhancing the utilization of the visible part of the solar spectrum. Based on this invention, novel photocatalysts that selectively sequester heavy metal ions and convert them to readily recoverable metallic forms will be developed, creating new technology for heavy metal removal from contaminated ground waters and aqueous waste streams from DOE and industrial operations. The pure metals deposited on the TiO(2) surface could be recovered or used directly as high surface area metallic catalysts. Selective reduction and recovery of various metals (Pb(+2), Ni(+2), Cd(+2), Cu(+2), Zn(+2), Cr(+6), U(+6), Pu(+6), Hg(+2)) and simultaneous removal of metals and organics will be investigated. This project pursues two main directions: 1) optimization of the photocatalyst by focusing on the charge-separation mechanism and electron-transfer reactions; and 2) optimization of the process including reactor design, treatment conditions, and catalyst regeneration.

Argonne National Laboratory
9700 South Cass Avenue
Argonne, IL 60439

8. Photorefractive Liquid Crystals: New Materials for Energy-Efficient Imaging Technology

Gary P. Wiederrecht
Chemistry Division
630/252-6963

Funding Profile
Date Started: February 15, 1995
Anticipated Duration: 3 Years

FY 95 - $320,000
FY 96 - $300,000
FY 97 - $289,000

This project will develop a new class of materials that will be used to produce energy-efficient image processing micro-devices. These materials will exploit the photorefractive effect, a light-induced change in the refractive index of a nonlinear optical material that results from photo generation of a space charge field caused by directional charge transport over macroscopic distances within a solid. Both frequency and phase information contained in light that has passed through a distorting medium can be recovered noise-free using photorefractive materials. The only high quality photorefractive materials commercially available today are expensive single crystals of inorganic materials such as barium titanate. This project will develop a completely new approach that combines cheap, easily processed organic materials with a built-in method of achieving the solid state order necessary to achieve photo refractivity comparable to that seen in inorganic crystals. The new approach uses organic molecules that undergo a phase transition above ambient temperatures to a liquid crystalline phase. Self-ordering in the liquid crystalline phase, followed by cooling to an ordered molecular solid, will impart both good optical nonlinearity and directional photoconductivity to thin solid films of these materials. These solid films have the potential to possess greater photorefractive sensitivity and faster response times than any material developed to date. The liquid crystals will be based on easily oxidized, disc-shaped organic molecules that are known to have liquid crystalline phases. The specific materials will be derivatives of triphenylenes, coronenes, porphyrins, and phthalocyanines. These molecules can be used to achieve the macroscopic order and good photoinduced charge generation characteristics that are required of high quality photorefractive materials for application throughout the visible and near-infrared spectral regions. Intrinsically asymmetric, nonlinear optical molecules, e.g. a chiral p-nitroaniline derivative, will be attached to the disc-shaped molecules and oriented in the liquid crystalline phase so as to maximize the nonlinear susceptibility of the material. Optical studies on the resulting solids will be utilized to verify the existence of photo refractivity and to accurately characterize the materials. Several device applications will be demonstrated.

Auburn University
Auburn University, AL 36849

9. Energy Related Applications of Selective Line Emitters

M. Frank Rose
Space Power Institute
334/844-5894

Funding Profile
Date Started: December 1, 1994
Anticipated Duration: 3 Years

FY 95 - $291,000
FY 96 - $254,000
FY 97 - $266,000

Infrared heat sources are used extensively for many processes in industry. From initial work, it appears feasible to develop intense infrared sources based upon electronic transitions in compounds of the rare earths, which tend to radiate efficiently at discrete wavelengths rather than a continuum. This project is aimed at conducting the basic and exploratory research that will allow the development of high intensity, discrete frequency infrared sources that are custom tailored to specific industrial processes. This will be accomplished by investigating and characterizing the emissive properties of the rare earths in inert forms such as oxides, borides, carbides, or nitrides. The Center for the Rare Earth Elements at the DOE Ames Research Laboratory will be used as the source of information for selection of suitable rare earth elements and compounds. Fibrous inert compounds of the rare earths will be formed as necessary. Oxide fibers can be formed by soaking activated carbon fibers in a suitable liquid compound of the rare earth, such as a nitrate of the material. Since activated carbon fibers can be greater than 70% porous, a substantial fraction of the liquid can be absorbed for suitable processing. The composite materials are formed into a paper with minor additions of cellulose using standard paper-making technology. Subsequent heating in a reducing atmosphere removes the cellulose and carbon, and forms essentially a pure metallic shell, mimicking the size of the activated carbon precursor. The final dimensions of the rare earth oxide fiber are determined by the initial dimensions of the precursor material. Successful samples will be characterized for strength, flexibility, and lifetime at temperature. Large area radiators for specific frequencies will be constructed and evaluated with the cooperation of an industrial affiliate.

University of California, Los Angeles
Los Angeles, CA 90024-1547

10. Characterization of a High Power RF Plasma Dissociation for Processing Mixed Wastes

Alfred Y. Wong
Department of Physics and Astronomy
310/825-9531

Funding Profile
Date Started: November 1, 1996
Anticipated Duration: 3 Years

FY 96 - $300,000
FY 97 - $300,000
FY 98 - $300,000

UCLA is investigating a plasma technology for partitioning and concentrating the heavy (radioactive) materials present in mixed waste, while simultaneously dissociating hazardous wastes. The central concept behind this technology is the combination of an inductively coupled plasma dissociation without internal electrodes and an electromagnetic plasma centrifuge. This project is an experimental program to characterize the scaling of our high power, high throughput, electrode-less rf plasma dissociation. An extensive survey of past work has resulted in a program to advance our current research device to one that could be combined with the centrifuge for experiments at the DOE Hanford site. The research consists of systematic gathering of key data on steady-state, high-density plasmas, produced at atmospheric pressure, using comprehensive physical and chemical diagnostic techniques. The observations will be analyzed within the context of disposing of toxic, hazardous, and radioactive wastes. The scaling laws of plasma temperature and density with applied rf power, size of the dissociator, carrier gas composition and pressure will be addressed. Through the use of laser interferometry, visible and infrared emission spectrometry, laser-induced fluorescence, local rf field, density and temperature measurements with water cooled probes, and a fully computerized GC/MS, the proposed studies will elucidate the science of plasma confinement by rf fields and vortex flows and non-equilibrium thermodynamics. The present device already demonstrates the effective dissociation of gas, liquid and solid samples. What is needed is the understanding of how this is accomplished through an overview of performance data and computer modeling of particle dynamics during dissociation. A well-tested atmospheric ion and neutral chemistry code will aid this process. Our experiments will be designed and built based on our present operating 50 kW dissociator, a fully computer controlled device. The research program will culminate in the design specification for a well-understood, research/proof-of-principle quality, 100 kW level rf plasma dissociator that can be interfaced with a plasma centrifuge currently being developed by UCLA and the DOE Hanford facility. This system will be tested with simulated mixed waste and can be transformed into a transportable waste disposer for localized (in laboratory) cleanup tasks. The project will interface with scientists at Hanford and Lawrence Livermore National Laboratory.

City College of City University of New York
Convent and 1389th Street
New York, NY 10031

11. Investigation of High Efficiency Multi Band Gap Multiple Quantum Well Solar Cells

Robert Alfano
Department of Physics
212/650-5532

Funding Profile
Date Started: April 15, 1997
Anticipated Duration: 3 Years

FY 97 - $225,000
FY 98 - $225,000
FY 99 - $225,000

This project will investigate and develop multiple quantum well (MQW) solar cells which are expected to reach much higher efficiency than that obtained from conventional bulk solar cells by reducing radiative and nonradiative relaxation processes through resonant tunneling. The maximum energy conversion efficiency of a conventional bulk solar cell is limited to less than ~33% because of its single band gap. Using a novel MQW-based solar cell with multi band gaps, one expects to enhance the maximum energy efficiency to ~72%. These high efficiency MQW solar cells have the potential of being widely used in compact computers, space power supplies, micro-scale motors, consumer products, home electronic devices, guide signs, and other renewable energy applications. In preliminary studies, we have measured carrier dynamics and band gap structures for GaAs, InP and their alloys, and calculated the resonant tunneling time and the barrier potential design criteria for achieving maximum energy conversion efficiency in MQW structures. Based on these measurements and calculations, we have designed several GaAs- and InP-based MQW solar cell structures which have been fabricated using the MBE facility at CCNY. The current-voltage (I-V) characteristics of the fabricated GaAs/AlGaAs MQW solar cells have been measured, and an enhancement of energy efficiency for the MQW solar cells over that of the conventional bulk solar cells has been observed. This project will enhance these studies and develop high efficiency multiband gap MQW solar cells. We will investigate resonant tunneling times for GaAs/AlGaAs and InGaAs/InP MQW structures to make sure that the resonant tunneling process dominates photocarrier collection. We will measure the I-V characteristics and investigate the energy efficiencies for GaAs/AlGaAs and InGaAs/InP MQW solar cells with different well and barrier configurations to select the best one. We will study multi-unit GaAs-and InP-based MQW solar cells to further increase the range of the band gaps and the energy efficiency. The target for the energy efficiency improvement is at least 150% for MQW solar cells over the conventional bulk solar cells. Industrial evaluations will be made by two companies (Applied Solar Energy in California and Plasma Physics in New York) during this project to determine the scientific and commercial potential of the MQW solar cells.

University of Colorado
Boulder, CO 80309-0347

12. Controlled Production of Cellulases in Plants for Biomass Conversion

Kathleen J. Danna
Department of Molecular, Cellular, and Development Biology
303/492-8735

Funding Profile
Date Started: June 15, 1996
Anticipated Duration: 3 Years

FY 96 - $162,000
FY 97 - $157,000
FY 98 - $164,000

Plant biomass, the most abundant renewable resource on earth, is a potential source of ethanol fuel, provided that the cellulose and hemicelluloses contained therein can be converted efficiently into fermentable saccharides for feedstock. The long-term objective of this project is to facilitate development of transgenic crop plants harboring cellulolytic enzymes that can be activated after harvest to produce a suitable, inexpensive feedstock. Using *Arabidopsis thaliana* for these pilot studies, we will generate transgenic plants that contain genes for an endoglucanase and an exocellobiohydrolase, both of which have high temperature optima. These thermostable enzymes are well suited for industrial applications, and their activities should be low at temperatures used for plant growth. Because we will provide each protein with a plant signal peptide fused to the amino terminus, the enzymes will accumulate in the apoplast, where they can be subsequently activated *in vitro* to degrade secondary and primary cell walls. If constitutive expression of these enzymes, under the control of the Cauliflower Mosaic Virus 35S promoter, is deleterious, we will confine expression of the genes to late periods of plant development by means of a senescence induced promoter, SAG12. We will: determine the effects of cellulase expression on plant growth and development and on cell wall structure and strength; determine the tissue and subcellular localization of the enzymes and the time course of expression; and evaluate the effectiveness of the enzymes to degrade endogenous cellulose *in vitro* under optimal enzyme reaction conditions.

University of Colorado
Boulder, CO 80309

13. Two-Dimensional Synthesis: Ultrathin Porous Membranes

Josef Michl
Department of Chemistry and Biochemistry
303/492-6519

Funding Profile
Date Started: December 1, 1993
Anticipated Duration: 3 Years (Project Completed)

FY 94 - $300,000
FY 95 - $300,000
FY 96 - $300,000

The objective of this research project is to synthesize and characterize an ultrathin fishnet-like sheet, suitable for application in molecular separations. This will be a new kind of heat-resistant organic-inorganic solid with a regular repeating two-dimensional structure, containing openings of a predetermined size. The first step will be the synthesis of a tentacle-carrying pillar-like monomer with three arms opposite to the tentacled end. Next, its molecules will be constrained by strong adsorption of the tentacles to a liquid-liquid interface, oriented with the pillar perpendicular to the surface and the arms parallel to it, at a distance of a little less that 10 angstroms. In the subsequent step, the arms of the monomer molecules will be cross-linked in two dimensions into a sheet composed of a regular covalent hexagonal lattice parallel to the surface. The polymerization will be monitored *in situ*. The lateral dimensions of the sheet will be maximized by a search for optimum reaction conditions. Neighboring sheet segments will be stitched together with relatively flexible threads to yield a large macroscopic piece of ultrathin membrane. The tentacles will then be clipped off, permitting desorption and removal of the net-like membrane from the surface. The construction will be completed by additional cross-linking to form a second hexagonal lattice on the side that previously carried the tentacles. The two hexagonal nets will thus be bonded into a single sheet through pillars located at well separated trigonal connector centers. The sheet will be about 15 to 20 angstroms thick, and will contain openings with a diameter of about 20 angstroms. The structure will be characterized by the techniques of surface science and its separatory properties will be tested. This will complete the proof-of-concept part of the project. The experience gained in the project will be used to design a second generation membrane for an actual industrial separation process, taking advantage of the flexibility available in the choice of the size of the openings, which can be chosen anywhere from nearly zero to about 40 to 50 angstroms in diameter, and in the choice of chemical functionalities at the rim of the openings.

Colorado State University
Fort Collins, CO 80523

14. A Novel Tandem Homojunction Solar Cell: An Advanced Technology for High Efficiency Photovoltaics

Bruce Parkinson
Department of Chemistry
970/491-0504

Funding Profile
Date Started: July 1, 1995
Anticipated Duration: 3 Years

FY 95 - $322,000
FY 96 - $268,000
FY 97 - $255,000

A material for the construction of a solar cell must meet a number of criteria to be suitable for large scale photovoltaic applications. It must be made up of abundant elements, which are environmentally benign, and when combined into a crystal have suitable electronic properties. The required electronic properties include a bandgap in the 1.1-1.8 eV range, high absorption coefficients to minimize the amount of material required, and high mobilities of photo generated carriers to facilitate the collection of these carriers. The semiconductor, ZnSnP(2), meets all of the above requirements. It is isoelectronic with the III-V alloy InGaP(2), but has the advantage, for photovoltaic applications, of not containing expensive and rare group III elements. In addition, this material does not contain toxic heavy metals such as are found in CdTe and CuInSe(2)/CdS thin film solar cells. The absorption coefficient for this material is also very high. The bandgap of ZnSnP(2) has the additional interesting and useful property of ranging from 1.24 to 1.66 eV, depending on the preparation conditions. Bulk crystal growth techniques have not yielded high mobility ZnSnP(2) but there is no *a priori* reason that the electronic properties of these materials cannot be as good as III-V materials, since very high mobilities were only achieved in III-V's after the development of modern epitaxial growth techniques. State-of-the-art metal-organic molecular beam epitaxy (MOMBE) will be used to grow epitaxial layers of ZnSnP(2) on lattice matched GaAs substrates. Studies of the order-disorder transition in the metal sublattice, using both optical and electrical techniques and especially solid state NMR to examine atomic scale local environments, will be conducted in order to find the conditions for preparing materials with various bandgap energies and to understand the basic chemistry and physics associated with this interesting order/disorder phase transition. When the conditions are established for preparing a material of a given bandgap, a "tandem homojunction" solar cell will be fabricated by variation of growth conditions in the MOMBE chamber in the appropriate way. This device should show significant efficiency advantages over a single material device or tandem heterojunction devices where lattice mismatch produces recombination-promoting interface states.

Drexel University
32nd and Chestnut Streets
Philadelphia, PA 19104

15. Plasma Energy Recycle and Conversion of Polymeric Municipal Solid Waste (MSW)

Richard Knight
Department of Materials Engineering
215/895-1990

Funding Profile
Date Started: December 15, 1996
Anticipated Duration: 3 Years

FY 97 - $143,000
FY 98 - $111,000
FY 99 - $115,000

This project will investigate the recycling of polymeric wastes using thermal plasma. A significant, valuable percentage of today's municipal solid waste (MSW) stream are polymeric materials, for which no economic recycling technology currently exists. This polymeric MSW is either incinerated, landfilled, or recycled into low-grade applications such as synthetic lumber. Thermal plasma technology is a potentially viable and economic means of recycling these materials more efficiently by converting them either back into monomers, which can be directed back into the polymer production cycle, or into other useful compounds which can be the starting materials for other chemical syntheses. A major limitation to the thermal plasma recycling of polymers is the lack of understanding of the reactions occurring during the process, of the quenching conditions necessary to "freeze" the products before complete pyrolysis occurs, and of the influence of process parameters on the reactions occurring and the yields obtained. This research will address this lack of understanding. This project has two goals: 1) To understand the chemical reactions occurring in a thermal plasma heated reactor during the rapid thermal processing (partial pyrolysis + rapid quenching) of polymeric materials; and 2) To determine and understand the effect of variations in thermal plasma reactor operating parameters (input power, gas flow rate/residence time, and quenching conditions) on the conversion of selected "model" polymeric materials to monomers or other organic compounds. These goals will lead to increased knowledge of chemical reactions under plasma conditions and to an enhanced understanding of the process parameters and reactor design required to carry out controlled depolymerization reactions. Model single material polymer systems, including polyethylene (PE), polypropylene (PP) and Polyethylene Terephthalate (PET) will be studied; analysis methods will include residual gas analysis, gas chromatography, and FTIR for the identification of chemical species; and thermal measurements of reactor operating parameters (temperature, enthalpy, etc.). This research offers the opportunity for a processing study to contribute directly to a strategically important, rapidly developing technology by depolymerizing polymeric wastes back to monomers or other precursor chemicals. Such a process should prove to be more economical than current landfilling and incineration.

Energy and Environmental Research Corp.
18 Mason
Irvine, CA 92718

16. Advanced Steel Reheat Furnace Development and Demonstration

Richard R. Koppang
714/859-8851

Funding Profile
Date Started: September 15, 1996
Anticipated Duration: 2 Years

FY 96 - $255,000

The steel industry is coming under stricter air emission regulatory control as the 1990 Clean Air deadlines are approached. Some of the higher emitting furnaces found in the steel industry are reheat furnaces, typically firing at between 50 and 500 MMBtu/hr, and annealing furnaces, typically firing at rates up to 100 MMBtu/hr. These furnaces tend to be inefficient, converting only 45 to 60% of the fuel usefully. Typical fuels fired are process off-gases and natural gas. This project intends to develop and commercialize an advanced steel reheat furnace which concurrently reduces NOx emissions by 50% while improving energy efficiency and productivity by up to 20%. The project will be conducted in three phases. In Phase I, a data base will be acquired on large, high temperature zoned furnaces found in the ceramics and steel service. Reference furnaces will be selected and rated for up to three appropriate applications. Computational modeling will be employed to parametrically estimate the efficiency benefits of the technology. In Phase II, design issues identified in Phase I will be systematically addressed and resolved through prototype component design and development. Pilot furnace tests and physical flow modeling will be performed as appropriate. In Phase III, a prototype system will be designed, constructed, and tested at a large, integrated steel mill.

Florida International University*
University Park
Miami, FL 33199

17. Association of N(2)-Fixing Cyanobacteria and Plants: Towards Novel Symbioses of Agricultural Importance

Miroslav F. Gantor
Department of Biological Sciences
305/348-2201

Funding Profile
Date Started: April 1, 1996
Anticipated Duration: 14 Months**
(Project Completed)

FY 96 - $162,000

The ever growing demand for nitrogenous fertilizers with their attendant energy cost and environmental complications, makes the alternative of biological N(2)-fixation increasingly attractive. Cyanobacteria comprise a significant portion of all N(2)-fixing microorganisms. Many can form symbiotic associations with diverse plants and fungi, but no case is known of a productive association of a cyanobacterium with an agriculturally important plant. Recently, we have demonstrated the ability of certain cyanobacteria to form intimate associations with wheat and rice and to penetrate the tissue of these plants. We will extend this work by addressing the following questions: 1) What is the most efficient method of introducing cyanobacteria into wheat? 2) What is the fate, location, and metabolic activity of cyanobacteria upon introduction into plants? 3) What is the cyanobacterial contribution to the nitrogen budget of the plant? And 4) What is the range of plants capable of forming such association? The fate and metabolic activity of cyanobacteria incorporated into plants will be monitored by a novel DNA-based method we have developed and by using cyanobacteria genetically tagged with genes encoding luciferase, an enzyme that produces luminescence. Different techniques of introducing cyanobacteria into plants, such as penetration via root, via stomata, co-culture of plant calli with cyanobacteria, and creation of nodule-like structures of plants and their colonization with cyanobacteria, will be considered. Cyanobacterial contribution to plant nutrition will be determined by measuring plant nitrogen content and (15)N incorporation. The results of these experiments may provide insight as to the requirements for exploiting N(2)-fixing cyanobacteria in the field and the benefits that may be expected.

*On September 1, 1997, this project was transferred to the University of Richmond under the direction of Professor Jeff Elhai, Principal Investigator.

**Includes 2 month no-cost extension. The total three-year funding for this project is $520,000.

General Electric Company
Schenectady, NY 12301-0008

18. Evaporation Through Tungsten to Achieve High-Rate Vapor Phase Processing of Intermetallics

Ann M. Ritter
Corporate R&D Center
518/387-7621

Funding Profile
Date Started: January 15, 1994
Anticipated Duration: 3 Years (Project Completed)

FY 94 - $291,000
FY 95 - $291,000
FY 96 - $318,000

The understanding of high-rate electron beam evaporation synthesis derived from this investigation will have significant impact on the ability to fabricate advanced designs of turbine blades, designs which cannot be produced by any state-of-the-art technology. Success in this project will make possible forming the complex cooling structure after the casting process, followed by a thin outer skin deposited by electron beam (EB) evaporation to create a double-wall. This structure, combined with composite materials developed specifically for the EB process, will provide long term efficiency improvements and enhanced service life. High-rate EB evaporation processes are currently difficult to control for deposition of complex alloys and intermetallics: fluctuations in power level and beam position can lead to large fluctuations in deposition rate and deposit chemistry. Modification of current practice of EB processes has been found to enhance chemistry uniformity and deposition rates through the addition of tungsten to the evaporation pool to permit much higher pool temperatures and stable pool dynamics. The objective of this research is to define optimum operating conditions for achieving economic deposition of controlled-chemistry, controlled-thickness Ni-base superalloys, NbTi-base metallic materials, and high strength, high temperature intermetallic phases. The approach will be to: evaluate process stability during prolonged evaporation through a tungsten-rich liquid pool; measure the effect of tungsten concentration in the pool on the evaporation process; characterize the influence of electron beam scan rate and scan pattern on the deposit chemistry and deposition rate; characterize the influence of the source temperature profile on deposit chemistry and deposition rate; determine evaporation conditions for Ni-base alloys containing Ta and Mo; and extend the electron beam evaporation-through-tungsten processing to higher melting intermetallic phases and NbTi-base metals.

University of Iowa
Iowa City, IA 52242-1219

19. Supported Molten Metal Catalysts. Development of a New Class of Catalysts

Ravindra Datta
Department of Chemical and Biochemical Engineering
319/335-1395

Funding Profile
Date Started: January 1, 1996
Anticipated Duration: 3 Years

FY 96 - $316,000
FY 97 - $322,000
FY 98 - $240,000

This project is concerned with the design and development of an entirely novel class of active and selective catalysts called supported molten-metal catalysts (SMMC), with a view to eventually replace some of the existing precious metal heterogeneous catalysts used in the production of fuels and chemicals. SMMC is based on supporting ultra-thin films of the relatively low-melting, inexpensive, and abundant metals and semimetals, from groups Ia, IIb, IIIb, IVb, Vb, and VIb elements, on porous refractory supports, much like supported microcrystallites of traditional solid catalysts. This technique could conceivably provide orders of magnitude higher surface area than that obtainable in conventional reactors containing molten metals in pool form while avoiding corrosion. These have so far been the chief stumbling blocks in the use of molten metal catalysts despite their higher selectivity and lower susceptibility to deactivation. While the SMMC technique can be applied to a large variety of reactions, we will initially concentrate on dehydrogenation and reforming reactions due to their commercial significance. Thus, dehydrogenation of methylcyclohexane and decalin and reforming of methylcyclopentane will be studied. These represent reactions of increasing complexity in catalytic reforming. The initial choice is tellurium-based catalysts including alloys, due to the very promising results obtained in preliminary screening experiments. Other catalytic formulations will also be tested. The activity, selectivity, and stability of the selected catalysts will be compared with the traditional Pt catalyst in differential packed-bed reactors. The commercial potential of the developed catalysts will be explored.

Johns Hopkins University
Baltimore, MD 21218

20. Ultrasonic and Dielectric Noninvasive Diagnostics for Sintering of Ceramic Composites

Moshe Rosen
Materials Science Department
410/516-8678

Funding Profile
Date Started: December 1, 1993
Anticipated Duration: 42 Months
(Project Completed)*

FY 94 - $358,000
FY 95 - $342,000
FY 96 - $290,000

The potential advantages of using microwaves to process ceramics have been recognized for more than three decades. However, only during the last several years, the scientific and engineering communities have experienced an outburst of research in this area. Nevertheless, a profound understanding of how materials interact with microwaves during sintering is still lacking. Measurement of the dielectric and mechanical properties of a material during microwave processing in real-time can provide the necessary theoretical and experimental insight into understanding this interaction that can subsequently be applied for the optimization of microwave processing of materials. In the course of this project, *in situ*, nonintrusive diagnostics for microwave sintering of ceramic materials will be developed. The essence of this project is a specially designed system for ultrasonic and dielectric probes to be integrated within the microwave furnace. The ultrasonic data can be ultimately related to the densification process during sintering of ceramics, while the dielectric characteristics are connected to the absorption mechanism of the microwave energy by the ceramic material. Acquisition of such data during sintering will shed light on the sintering kinetics and its mechanism and, consequently, provide an understanding of the optimal sintering conditions needed to achieve maximum densification and the desired material properties. Furthermore, such data can be instrumental in developing predictive models for microwave sintering of ceramic materials.

*Includes 6 month no-cost extension

Lawrence Berkeley National Laboratory
Berkeley, CA 94720

21. Compact MeV Ion Implanter

Simone Anders
Plasma Applications Group
510/486-6745

Funding Profile
Date Started: February 15, 1994
Anticipated Duration: 3 Years (Project Completed)

FY 94 - $294,000
FY 95 - $319,000
FY 96 - $298,000

A new kind of MeV ion implanter will be developed, the distinguishing features of which will be its relatively small size and low cost. The heart of the device will be a novel kind of ion source by means of which high charge state ions will be produced, thereby allowing the production of high energy ion beams (1 MeV and above), using only modest accelerating voltages (one to several hundred kV). The ion source will be a repetitively pulsed vacuum spark source, and the implantation facility will thus also generate repetitively pulsed, large area, metal ion beams. By virtue of the relatively low voltages employed, the implanter will be much more compact and of much lower cost than present state-of-the-art facilities that employ singly charged ions and megavolt power supplies. From the perspective of new physics, a novel kind of ion source will be developed - vacuum arc ion sources have been developed but not vacuum spark ion sources, and it is in the latter that the highly stripped ions are to be found, yielding high energy at modest voltage. From the perspective of new technology, this is an entirely new approach to doing MeV ion implantation, making high energy surface modification techniques feasible for a vastly broader field of users than at present.

Lawrence Berkeley National Laboratory
Berkeley, CA 94720

22. Novel and Energy Efficient Co-Factor Regeneration for Enzymatic Catalysis

John B. Kerr
Energy and Environment Division
510/486-6279

Funding Profile
Date Started: May 15, 1997
Anticipated Duration: 3 Years

FY 97 - $336,000
FY 98 - $324,000
FY 99 - $310,000

Catalytic systems based on enzymes are potentially capable of altering the nation's energy picture through the use of alternative fuels and feedstocks. Their well-known selectivity can also aid in the reduction of pollution resulting from manufacturing processes and they have an important role to play in waste treatment and clean-up. Novel non-enzymatic regeneration reactions of co-factors, NAD+ and NADH, are urgently required to facilitate the introduction of oxido-reductase enzymes into industrial and environmental processes. The feasibility of efficient regeneration of NADH and NAD(P)H co-factors using bioorganometallic catalysts and electrochemical flow cells will be investigated. A study of (5-pentamethylcyclopentadiene)rhodium (Ligand)(Aqua) complex reactivity with NAD+ will be undertaken to discover the mechanism of, and hence, the structural features responsible for regiospecifc transfer of hydride to form the enzymatically active 1,4-NADH. A biomimetic membrane will be designed and synthesized to simplify downstream separation processes. The organometallic catalyst will be attached to electrodes via covalent bonding through the Cp* ligand to polyethyleneglycol-type polymers, cross linked appropriately to allow adherence of the membrane to the electrode and adequate access of the substrates to the catalysts. The cost-benefits of tethering the catalyst, the co-factor and/or the enzyme to the electrode will be measured for scale-up design and commercial operation. Electrochemical behavior of the catalysts will be fully characterized. Structures of the Cp* and nitrogen bases will be varied to modulate the electron density around the rhodium metal center and thereby alter the kinetics and stability of the catalyst. Turnover rates over 100/s and turnover numbers above 109 are desirable to apply the system in high volume/energy intensive processes. Less expensive organometallic centers will be investigated and the use of alternative photochemical or chemical energy delivery will be assessed.

Lawrence Berkeley National Laboratory
Berkeley, CA 94720

23. Blue-Emitting Devices Based on Gallium Nitride

Michael D. Rubin
Energy and Environment Division
510/486-7124

Funding Profile
Date Started: May 15, 1994
Anticipated Duration: 3 Years (Project Completed)

FY 94 - $319,000
FY 95 - $340,000
FY 96 - $332,000

The purpose of this project is to convert the recent breakthroughs in growth of gallium nitride (GaN) into practical ultraviolet and blue light emitting diodes and lasers. This technology is critical to national competitiveness in the development of the next generation of optoelectronic devices. Short-wavelength semiconductor devices based on GaN are needed for many important applications such as energy-efficient illumination, high-density optical data storage, flat-screen color displays, underwater communications, and high-temperature electronics. GaN is a III-V semiconductor with a direct bandgap of 3.4 eV in the ultraviolet. One of the principal technical problems that limits device applications has been achieving controllable p-type doping. The stoichiometry of the films was greatly increased using a reactive ion-beam process, thus eliminating the primary background donor concentration. Upon attaining threshold levels of conductivity and mobility, it was discovered that p-type conversion could be readily obtained by a variety of doping methods including ion implantation, diffusion and co-evaporation of Mg. The defect studies which guide the improvements in the growth process will be continued. This process, along with specialized ion beam technology, will be transferred to Hewlett-Packard where it will be reproduced in a large-scale commercial growth system. Simultaneously, fabrication of light-emitting devices will begin, using current materials, in cooperation with Hewlett-Packard.

Lawrence Berkeley National Laboratory
Berkeley, CA 94720

24. Combinatorial Synthesis of High Tc Superconductors

X. D. Xiang
Materials Science Division
510/486-6640

Funding Profile
Date Started: March 15, 1996
Anticipated Duration: 3 Years

FY 96 - $144,000
FY 97 - $250,000
FY 98 - $250,000
FY 99 - $106,000

Currently, there is a tremendous interest in materials such as high temperature superconductors, organic conductors, permanent magnets, nonlinear optical materials and zeolites. However, even though the properties of such materials have been extensively investigated, few general principles have emerged that allow one to predict the structures of new materials with enhanced properties. Consequently, the discovery of such materials remains a time consuming and rather unpredictable trial and error process made even more difficult by the increasing complexity of modern materials. The question arises whether there is a more efficient and systematic approach to search through the largely unexplored universe of ternary, quaternary, and higher order solid state compounds, in order to discover materials with novel electronic, optical, magnetic or mechanical properties. We will develop a new approach to materials discovery that will significantly increase the rate at which novel materials are discovered as well as increase our ability to correlate physical properties with structure. Specifically, we will develop the ability to rapidly synthesize and analyze large libraries, or collections, of solid state materials for specific electronic, magnetic, optical and structural properties. The aim of this project is twofold: 1) to develop the technology to the point where it can be used effectively for materials discovery; and 2) to apply the technology to the discovery of new superconducting materials.

Lawrence Livermore National Laboratory
Livermore, CA 94550

25. Converting Agricultural Waste to Automotive Fuels: Electrochemical Production of Nitromethane

Thomas T. Coburn
Analytical Science Division
510/423-1316

Funding Profile
Date Started: March 15, 1997
Anticipated Duration: 2 Years

FY 97 - $270,000
FY 98 - $264,000

This project will develop a novel electrochemical means for producing nitromethane from acetic acid. The process is grounded in chemistry already investigated at Lawrence Livermore National Laboratory (LLNL) by the authors and is based on conversion of inexpensive organic feedstocks (e.g., acetic acid) to nitromethane or its analogs in a highly oxidizing nitric acid media. Nitric acid is circulated in a closed-loop system, and the highly oxidizing environment is maintained by continuous electrochemical oxidation/re-oxidation of a transition-metal "mediator." The proposed research will elucidate the electrochemical/chemical reactions and optimize the process chemistry and engineering aspects of the novel nitromethane production unit. Applicability of the technology to the production of various nitromethane analogs, such as an environmentally acceptable refrigerant and some precursors for the manufacture of explosives will be investigated. The potential economic impact of this project is enormous. The proposed method of production would lower the cost of nitromethane as a clean-burning automotive fuel to a level that would be competitive with the cost of current fuel components.

Lawrence Livermore National Laboratory
Livermore, CA 94550

26. Thermoelectric Quantum Wells

Joseph C. Farmer
510/423-6574

Funding Profile
Date Started: January 15, 1994
Anticipated Duration: 3 Years (Project Completed)

FY 94 - $350,000
FY 95 - $350,000
FY 96 - $350,000

Solid state thermoelectric devices have no moving parts and can be used to convert heat directly into electricity. Such devices can also be used as chlorofluorocarbon (CFC)-free refrigerators, provided that an external voltage is applied. Unfortunately, thermoelectric devices are not as efficient as their mechanical counterparts. However, theoretical physicists at the Massachusetts Institute of Technology have recently used quantum mechanics to design a new class of thermoelectric materials that may improve the efficiency (figure of merit) of thermoelectric devices to a point where they are competitive with conventional internal combustion engines and CFC-based refrigerators. Process technology developed at Lawrence Livermore National Laboratory for the fabrication of x-ray optics is now being used to synthesize these new multilayer thermoelectric thin films. Multi layers are being made by alternately sputtering quantum well and barrier layers onto a moving substrate from dual magnetrons. A number of multilayer films, including high-temperature Si(0.8)Ge(0.2)/Si and low-temperature Bi(0.9)Sb(0.1)/PbTe(0.8)Se(0.2), are being synthesized and evaluated. This research can lead to new materials and devices.

Lawrence Livermore National Laboratory
Livermore, CA 94550

27. Porous Carbons: Controlling Structure, Composition and Performance

Tri D. Tran
Chemistry and Materials Science Department
510/422-0915

Funding Profile
Date Started: March 15, 1994
Anticipated Duration: 42 Months
(Project Completed)*

FY 94 - $335,000
FY 95 - $355,000
FY 96 - $374,000

This research examines the synthesis and processing conditions necessary to tailor the local structure and composition of porous carbons for potential applications in energy storage devices (i.e., batteries, capacitors). Carbon aerogels are being formed from resorcinol-formaldehyde and phenolic-furfural precursors. These porous carbons have low electrical resistivity, an ultra fine pore size distribution, high surface area (400 to 1100 square meters per gram, roughly the size of one or two basketball courts), and a solid matrix composed of interconnected particles or fibers. Preliminary data show that these materials are attractive electrodes for double layer capacitors. Carbon foams derived from the phase separation of polyacrylonitrile/solvent mixtures are being investigated as lithium intercalation anodes for rechargeable lithium-ion batteries. These carbon foams differ from aerogels in that they have much larger pore sizes and one or two orders of magnitude lower surface area. High capacity and good cycle ability are observed during lithium intercalation experiments. These materials can potentially lead to new batteries with energy densities that are approximately four times greater than conventional nickel-cadmium batteries. In summary, this research project investigates sol-gel polymerization of multi functional organic monomers, the phase separation of polymer/solvent mixtures, the formation of porous composites, intrinsic chemical doping, and pyrolysis in controlled atmospheres. A variety of characterization tools are being used to study the structure and properties of porous carbons. The overall objective is to develop a fundamental understanding of how morphology, chemical composition, and local order affect the electrochemical performance of porous carbons. The potential payoff from this research is the development of new energy storage devices with superior performance.

*Includes 6 month no-cost extension

Los Alamos National Laboratory
Los Alamos, NM 87545

28. Conversion of Atmospheric and Effluent Carbon Dioxide to Methanol via High Temperature Photolysis

Reed J. Jensen
505/667-0187

Funding Profile
Date Started: May 15, 1995
Anticipated Duration: 3 Years

FY 95 - $200,000
FY 96 - $300,000
FY 97 - $250,000

The purpose of this project is to gather data to support an evaluation of a proposed process for the conversion of atmospheric and effluent CO(2) to methanol via high temperature, solar photolysis. The underlying principle is that once CO(2) is converted to CO, it is a simple matter to convert it to methanol. Recent work in Europe has shown the existence of previously unknown, bent, excited states of CO(2). It is now evident that any form of vibrational energy enables the transition to these states through symmetry effects and enhanced Frank-Condon factors. The states lie much lower than the well known dissociative states near 9 eV. The absorption cross sections for transitions to these states will be measured at temperatures up to 2800 K. The approach is to employ an existing hot gas cell to measure light absorption and oxygen production. A laser system will provide violet and blue wavelengths important to the central idea of this proposal. Favorable basic data from these measurements could lead to an effective process for reducing atmospheric CO(2) and decreasing oil imports.

Los Alamos National Laboratory
Los Alamos, NM 87545

29. Seismic Stimulation of Oil Production in Depleted Reservoirs

Paul Johnson
GeoEngineering Group
505/667-8936

Funding Profile
Date Started: December 15, 1995
Anticipated Duration: 3 Years

FY 96 - $300,000
FY 97 - $300,000
FY 98 - $300,000

This project will explore an unproven method for increasing energy production and economy: the stimulation of oil reservoirs by seismic waves. We propose to identify and quantify the importance of critical experimental variables that can enhance oil production in the presence of elastic wave stimulation. Our work will proceed in two stages: exploratory R&D and field demonstration. In the first stage, we will perform scaled laboratory experiments on typical formation rocks. We will determine wavefield parameters that cause changes in relative permeability of oil for different oil-to-water ratios and changes in residual oil saturation for simulated waterflood tests. We will also perform theoretical modeling and laboratory experiments as needed to study physical mechanisms for flow enhancement due to wave stimulation. In the second stage of work, we will collaborate with four major oil companies, Texaco, Marathon, Amoco and Phillips Petroleum, to perform stimulation tests in oil fields with well characterized physical properties and production histories. The laboratory and field tests will be partially supported by contributions from our industrial collaborators. Results of our laboratory and theoretical work will be used to design the field experiments. We intend to demonstrate the potential usefulness of wave stimulation techniques for enhancing oil production. Our work could provide strong incentives to the oil industry to further develop this technology for routine implementation in secondary recovery procedures.

Los Alamos National Laboratory
Los Alamos, NM 87545

30. Magnetically Enhanced Thermoelectric Cooling

Albert Migliori
Materials Science and Technology Division
505/667-2515

<u>Funding Profile</u>
Date Started: March 15, 1996
Anticipated Duration: 3 Years

FY 96 - $250,000
FY 97 - $250,000
FY 98 - $250,000

Cryogenic solid-state refrigerators based on the Ettinghausen effect can provide vastly superior performance to Peltier devices, opening up new markets in electronics and in superconductor-, and medical applications. Surprisingly, this most effective of solid-state cryogenic refrigeration processes is not being studied at present. Yet it is much less restrictive in the possible materials that can be used, is simpler to construct (even noting that a small permanent magnet must produce a field at the device), and has already achieved lower temperatures than Peltier coolers, the only devices presently under investigation. Recent discoveries of new hybridization-gap semi-conductors and semi-metals, and the commercial availability of high-strength $Nd(2)Fe(14)B$ permanent magnets, open the way for development of new ultra-high-performance, all solid-state Ettinghausen refrigerators. We will initiate studies of such coolers using modern materials to engineer the world's best solid-state cryocooler.

Louisiana State University
Baton Rouge, LA 70803-7303

31. Combining Steam-Methane Reforming, Water-Gas Shift, and CO(2) Removal in a Single-Step Process for Hydrogen Production

Douglas P. Harrison
Department of Chemical Engineering
504/388-3066

<u>Funding Profile</u>
Date Started: March 15, 1997
Anticipated Duration: 3 Years

FY 97 - $124,000
FY 98 - $111,000
FY 99 - $114,000

The objective of this project is to investigate a number of options for improving the steam-methane reforming process for hydrogen production. It has been recognized for several decades that an improved process is theoretically possible if some of the processing steps, now conducted separately, are combined. However, the identification of a practical approach to implementation of the improved process has proved to be elusive. This proposal identifies a catalyst and processing conditions that may allow the reforming and shift reactions to be conducted in the presence of a carbon dioxide acceptor (lime).

If successful it will identify a practical approach for realizing the benefits of the combined process.

Louisiana State University
Baton Rouge, LA 70803-7303

32. Reducing Energy Consumption and Pollution in Plastic-Manufacturing Processes: Phase Behavior Roots of Fouling Phenomena that Cause Energy and Product Waste

M. Radosz
Department of Chemical Engineering
504/388-1750

Funding Profile**
Date Started: September 15, 1996
Anticipated Duration: 3 Years

FY 96 - $122,000
FY 97 - $122,000
FY 98 - $122,000

The overall goal of this project is to understand the phase behavior of ethylene copolymers in compressible fluid streams, such as copolymer solutions in supercritical and near critical fluids. Such understanding is needed to develop new plastic-manufacturing processes that are less energy intensive, and produce less pollution and less waste product. Specifically, such understanding is needed to be able to control undesirable phase transitions and, hence, eliminate the root cause of fouling phenomena in pipelines, reactors and separators. This is in contrast to mitigating the fouling consequences using specially treated surfaces and additives. The approach is a synthesis of experiment and thermodynamic modeling. The experiments will be aimed at accurate phase transition data for well-characterized model polyolefin systems. The thermodynamic modeling will be aimed at predicting such phase transitions. The basis for this approach is a series of preliminary but promising experimental and computational results with an equation of state, referred to as the copolymer SAFT (statistical associating fluid theory). The copolymer SAFT should explicitly account for the effects of micro structure on the thermodynamic properties of copolymers. This has never been done before and will impact the way we characterize very large, structured molecules. The objectives proposed for this project will concern a specific system of ethylene copolymers and small olefins. The focus will be on the effect of branchiness (hence crystallinity) and molecular weight on the phase transitions that induce undesirable fouling phenomena.

**Budgets include funding from Basic Energy Sciences' Materials Sciences Division

Massachusetts Institute of Technology
Cambridge, MA 02139

33. Superconducting Bitter Magnets

Leslie Bromberg
Plasma Fusion Center
617/253-6919

Funding Profile
Date Started: May 1, 1993
Anticipated Duration: 4 Years (Project Completed)*

FY 93 - $300,000
FY 94 - $300,000
FY 95 - $300,000

A novel process for manufacturing high temperature superconducting magnets using thick-film superconducting material on structural plates is described. This technique is similar to that used in constructing Bitter magnets. The superconductor is manufactured in the required shape, avoiding the need to develop ductile wires. The structural metal plate serves as the material as well as the quench protector. A dielectric with high electrical resistivity is placed between the conductor and the metal plate (copper, aluminum, composite materials). This method can be utilized for manufacturing solenoidal, toroidal, saddle, and other types of magnets with both high-T(c) and low-T(c) superconductors. This project will address issues faced in this type of magnet construction (quench protection, materials compatibility, stability, and cooling). A theoretical program to gain understanding of these issues will be carried out. Experiments will be conducted to determine the feasibility of manufacturing magnets using this technique. Several methods for manufacturing the superconductor will be tested. Interaction with the manufacturers to improve the performance of superconducting materials for this application will be maintained. It is expected that in the final phase of this program, magnets will be constructed and tested. A team arrangement between the Plasma

Fusion Center at the Massachusetts Institute of Technology (MIT) and the Superconductivity Technology Center at the Los Alamos National Laboratory (LANL) has been established.

*Includes 12 month no-cost extension

University of Michigan*
Ann Arbor, MI 48109-2099

34. Tunable Femtosecond UV Light Source Using a Novel Frequency Upshift Technique

Henry C. Kapteyn
Center for Ultrafast Optical Science
313/763-0573

Funding Profile
Date Started: July 15, 1996
Anticipated Duration: 1 Year (Project Completed)

FY 96 - $172,000**

The goal of this project is to implement a new approach for producing ultra short light pulses at ultraviolet to extreme-ultraviolet wavelengths. An intense light pulse can be used to create a moving ionization front; light can be reflected from this front and experience a relativistic Doppler upshift. Two recently-developed technologies now make it possible to create tunable light pulses of unprecedented short duration using this technique. First, the recent development of small-scale terawatt femtosecond laser systems makes it possible to create an extremely abrupt moving ionization front, using the process of multi photon ionization. Second, recently-developed techniques have resulted in the generation of single-optical-cycle duration pulses in the far-infrared. It is shown herein that it is possible to upshift such pulses to optical and shorter wavelengths while still retaining nearly single-cycle duration. This way, pulses of 1-5 femtoseconds duration in the UV to XUV region of the spectrum can be created.

*This project was started on April 19, 1993, at Washington State University; it was transferred to the University of Michigan as a result of Professor Kapteyn's relocation.

**The total three-year funding for this project is $445,000.

University of Michigan
Ann Arbor, MI 48109

35. Feasibility of a Novel Approach for Fast, Economical Determination of Radiation Damage in Nuclear Reactor Cores

Gary S. Was
Department of Nuclear Engineering
313/763-4675

Funding Profile
Date Started: November 1, 1992
Anticipated Duration: 4 Years (Project Completed)*

FY 93 - $156,000
FY 94 - $145,000
FY 95 - $149,000

The objective of this project is to determine the feasibility of using proton irradiation as a radiation damage tool, resulting in order-of-magnitude savings in time and cost over current methods to study radiation damage. The feasibility will be established through the application of proton irradiation to the determination of the mechanism of irradiation assisted stress corrosion cracking (IASCC) in light water reactors (LWRs). The technique is ideally suited to this major industry problem. The emphasis of the technical program will be on the role of grain boundary chemistry and micro structural changes on IASCC. High energy proton irradiation has recently been shown to produce grain boundary segregation of the major alloying elements and impurities, and a micro structure that is comparable to that produced by neutron irradiation in a fraction of the time and at a fraction of the cost. This project is designed to uncover the effects of grain boundary impurity segregation, chromium depletion, and the irradiated micro structure on IASCC. It involves both experimental and computational efforts that have been developed in our laboratory. The plan also calls for investigation of the dose, dose rate, temperature and injected hydrogen effects and comparison with available neutron irradiation data. The combination of micro structure characterization with its dependence on critical irradiation parameters will provide both a better understanding of the role of irradiation in the mechanism, as well as an assessment of the feasibility of using proton irradiation to study neutron irradiation in LWR cores. Collaborations with industry and national laboratories have been established to exchange materials that will allow us to benchmark results of proton irradiation against neutron irradiation and to determine the irradiation conditions that produce the best match. Because the time and cost involved in these experiments is a small fraction of that required for neutron irradiation, the technique will provide a more cost-effective and time-efficient method of studying radiation change in core structures and in assessing new materials.

*Includes 12 month no-cost extension

University of Minnesota
Minneapolis, MN 55455

36. Injection Molding of Plastics from Agricultural Materials

Mrinal Bhattacharya
Department of Agricultural Engineering
612/625-5234

Funding Profile
Date Started: January 1, 1996
Anticipated Duration: 3 Years

FY 96 - $166,000
FY 97 - $169,000
FY 98 - $172,000

In the last few years there has been a renewed interest in the development of materials that mimic plastics and have a significant component of agricultural commodities. For example, these materials could be a blend of starch and/or protein and a synthetic polymer. The goal for such materials is two-fold. First, the materials can be processed into end products having acceptable physical and chemical properties pertaining to their end use. Second, increased environmental friendliness of the product may open an avenue for increased usage of farm commodities and other renewable resources. The presence of the synthetic polymer is needed to impart desirable physical properties, for example, insensitivity to moisture, or tensile- and impact strength. While the biodegradability of the product depends on the degradability of the synthetic material, the presence of a large agricultural component in the blend (60 to 70% or more) is expected to reduce the environmental impact of 'plastic' material. Moreover, the increased use of an agricultural component is expected to add significant value to the large surplus of farm commodities that currently exists in the United States. The processing of blends of these materials remains a largely unexplored area. Most plastic parts are produced by extruding and then injection molding. Injection molding, a widely used method of polymer processing, is characterized by high production rates and accurately sized products. Yet, other than in terse citations in patents, injection molding of starch-based plastics has not been discussed in the scientific literature. A thorough understanding of the molding process is necessary to produce products of the required quality at the lowest possible cost. Furthermore, the fact that we are concerned with a blend (as opposed to a homopolymer) complicates matters significantly. The presence of weld lines in injection-molded articles made from homopolymers is known to limit the use of plastic materials. This problem is compounded in the case of polymer blends. During the flow process, a polymeric material undergoes simultaneous mechanical and thermal influences and changes of state. Also, depending on the morphology, the flow process will introduce orientation, residual stresses, and shrinkage in injection-molded products that affect the physical properties and dimensional stability of the finished products.

National Renewable Energy Laboratory
1617 Cole Boulevard
Golden, CO 80401-3393

37. PV-Powered, Electrochromic Windows

David K. Benson
Basic Sciences Division
303/384-6462

Funding Profile
Date Started: February 15, 1994
Anticipated Duration: 3 Years (Project Completed)

FY 94 - $330,000
FY 95 - $330,000
FY 96 - $330,000

This project will develop a retrofit window treatment for architectural windows. The window treatment will be a combination of thin-film photovoltaic cells and an electrochromic coating, both deposited onto a flexible polymer film. The coated polymer film will be applied to the interior surfaces of existing building windows and used to modulate the solar transmittance into the building thereby providing automatic solar-gain control and day lighting control functions which will reduce heating, cooling, and lighting energy usage in the building. The selfpowered window obviates the need for costly electrical wiring. This kind of "smart" window covering has the potential to balance the performance of the window, giving it a net energy benefit. It has been predicted to be able to reduce the cooling power demand of a south-facing window in a climate such as southern California by about 40% and to have similar benefits in other locations. A large fraction of the billion square meters of existing building windows in the U.S. could benefit from this kind of treatment. At present, an estimated 1 to 1.5% of the total cooling energy need in buildings and 10 to 30% of the peak electric utility power demand is caused by windows amounting to about a 1500 MW increase in electric utility peak electric power demand each year due to new windows at a national operating cost of about $10 billion. New photovoltaic and electrochromic coating designs and new processes for their deposition onto flexible polymer substrates will be developed in this project.

National Renewable Energy Laboratory
1617 Cole Boulevard
Golden, CO 80401-3393

38. Efficient Energy Up-Conversion of Infrared to Visible Light at Semiconductor Heterojunctions

Hyeonsik M. Cheong
303/384-6484

Funding Profile
Date Started: March 15, 1997
Anticipated Duration: 3 Years

FY 97 - $268,000
FY 98 - $243,000
FY 99 - $253,000

A recently-discovered energy up-conversion phenomenon in semiconductor heterostructures will be studied. This phenomenon could be used to make light emitting devices that emit a wide range of colors and even multiple colors or white light. Possible applications for such devices are energy-efficient multi-color displays or a white light source to replace incandescent lamps in some areas. The principal advantage of such devices would be that multiple elements of these up-conversion structures with different emission colors, as well as the excitation source for the up-conversion, can be grown *monolithically* on a single wafer. When GaAs/AlGaInP(2) heterostructures are excited with a near-infrared laser at 1.52 eV (815 nm), electrons and holes are created in the lower-band-gap material (GaAs). Some of these electrons and holes are excited to the higher-band-gap material (AlGaInP(2)), and then radiatively recombine at the band gap of AlGaInP(2), giving up-converted luminescence in red, orange, or green depending on the aluminum concentration in the AlGaInP(2) alloy. The objective of the study is to demonstrate the feasibility of the devices utilizing this novel phenomenon of up-conversion. In order to achieve this, we will examine various semiconductor heterostructures to find the optimal semiconductor heterostructure system that give the highest up-conversion efficiency. This will require sophisticated band-structure engineering using a number of different semiconductors including GaAs, AlGaAs, GaInP(2), and AlGaInP(2). We will also perform a systematic study of the mechanism for this up-conversion using both cw and ultrafast optical spectroscopies. The final phase of this project will be devoted to realization of a prototype device in which either vertical-cavity surface-emitting laser structure or a pn junction is used to excite up-conversion luminescence.

National Renewable Energy Laboratory
1617 Cole Boulevard
Golden, CO 80401-3393

39. Hot Carrier Solar Cells

Mark C. Hanna
Basic Sciences Division
303/384-6620

Funding Profile
Date Started: February 15, 1994
Anticipated Duration: 46 Months*

FY 94 - $330,000
FY 95 - $330,000
FY 96 - $330,000

This project is focused on the development and understanding of a new kind of high efficiency solar cell, called a Hot Carrier Solar Cell (HCSC), which may have the potential to double the maximum efficiency of conventional solar cells. The ultimate thermodynamic conversion efficiency of an optimized HCSC is 66%, compared to 31% for an optimized conventional single bandgap solar cell. This project explores a new approach for increasing the efficiency of solar cells by attempting to utilize the excess kinetic energy of higher energy (hot) carriers generated by the absorption of high energy photons in the solar spectrum. Normally, the excess kinetic energy of hot carriers created by absorption of solar photons in photovoltaic cells is converted to heat and is thus unavailable for useful work. The HCSC employs a new type of semiconductor structure (called a superlattice) to absorb the solar photons and to inhibit hot carriers from cooling in the photovoltaic device. Bandgap engineering techniques will be used to control important physical properties of the superlattice, such as the hot carrier energy loss rate, hot carrier mobility, and the absorption threshold. Hot carriers from the superlattice region are collected in high bandgap contacts to produce a higher photovoltage. With this combination, the photo current and photovoltage of the cell can be separately controlled and optimized, unlike the conventional p-n photovoltaic cell where the photo current and photovoltage are coupled. The HCSC is fabricated from Group III-V semiconductor compounds and alloys grown by low pressure organometallic chemical vapor deposition. This project will synthesize HCSCs, measure their performance and properties, compare them to appropriate conventional solar cells, and develop a theoretical model for predicting the device characteristics of the HCSC.

*Includes 10 month no-cost extension

National Renewable Energy Laboratory
1617 Cole Boulevard
Golden, CO 80401-3393

40. Single-Wall Carbon Nanotube Materials for Purification of Natural Gas

Michael J. Heben
Center for Basic Sciences and Advanced Concepts
303/384-6641

Funding Profile
Date Started: May 15, 1997
Anticipated Duration: 2 Years

FY 97 - $316,000
FY 98 - $255,000

About one-third of our Nation's natural gas reserves and undiscovered/undeveloped resources are an unusable, low-quality grade owing to excessive quantities of carbon dioxide, nitrogen, water and hydrogen sulfide and must be purified prior to use. The use of carbon single-wall nanotube (SWNT) materials for extracting methane from highly impure streams is the focus of this project. This novel approach will utilize the unique adsorption properties of SWNTs to differentially remove impurities from natural gas. Preliminary research has shown that both CO(2) and H(2)O are preferentially adsorbed onto SWNT-containing materials versus CH(4). This discovery is non-intuitive and provides the basis for the application of SWNT materials into separations technologies. SWNT materials will impact both adsorption and membrane approaches to natural gas purification. First, the use of SWNT powders and films as adsorbents in pressure swing adsorption separation technologies will be investigated. Second, nanotube/alumina membrane composites will be fabricated which selectively transmit gaseous species based on differences in molecular size and polarizability. Synthetic manipulation of the membrane structures should provide control over equilibrium adsorption, surface diffusion and molecular sieving phenomena enabling the unique opportunity to impact the separations industry in a timely fashion.

National Renewable Energy Laboratory
1617 Cole Boulevard
Golden, CO 80401-3393

41. Atomic and Nanoscale Engineering of Thermophotovoltaic Semiconductors Using Scanning Probe Microscopy Techniques

Lawrence L. Kazmerski
Photovoltaics and Basic Sciences Division
303/384-6604

Funding Profile
Date Started: July 10, 1994
Anticipated Duration: 41 Months*

FY 94 - $177,000
FY 95 - $552,000
FY 96 - $315,000

This project uses scanning probe microscopes for the atomic-scale engineering of semiconductors leading to advances in understanding their improvement, and their use in energy-conversion thermophotovoltaic (TPV) structures and devices—cells designed to produce electricity from surfaces emitting radiation in the 1400 to 2000 K range. This project consists of three interrelated segments: 1) preparation of selected GaInAs and GaInAsP alloy surfaces having suitable compositions; 2) use of modern electronic structure theory to predict the properties of these semiconductor surfaces before and after atomic-scale engineering takes place and to provide guidance for the experiments; and, the central and primary activity, 3) evolution of the novel atomic processing microscope to image, process (including atom removal and placement), and characterize these semiconductors with the same nanoscale spatial resolutions and to produce nanometer-scale optimized TPV structures for the next generation of these energy conversion devices. These atomic-scale investigations involve the manipulation of atoms in order to study the fundamental defect properties that limit both materials properties and device performance. This project provides the first atomic engineering directed toward these III-V materials. It further provides fundamental information of the nature of defects, their electro optical properties and the ability to electronically heal them with intrinsic and extrinsic atomic species. This project links events on the atomic scale to the current understanding of semiconductor surface and interface physics. The project provides first-time characterization of the electro optical properties of TPV semiconductors in compositional ranges not previously investigated. This information is used to demonstrate optimized next-generation TPV structures that will lead to highly efficient cells for energy applications.

*Includes 5 month no-cost extension

National Renewable Energy Laboratory
1617 Cole Boulevard
Golden, CO 80401-3393

42. Photochemical Solar Cells

Arthur J. Nozik
303/384-6603

<u>Funding Profile</u>
Date Started: January 15, 1995
Anticipated Duration: 3 Years

FY 95 - $150,000
FY 96 - $150,000
FY 97 - $150,000

Very high power conversion efficiencies (8-12%) for photochemical solar cells were reported in 1991. These solar cells consist of highly porous nanocrystalline films of TiO(2) (band gap=3.0 eV) that are sensitized to the visible region of the solar spectrum through adsorption of Ru-containing metal-organic dye complexes on the TiO(2) particle surface. This represents more than two orders of magnitude improvement in the power conversion efficiency of dye-sensitized semiconductor electrodes in a photochemical cell. A dye-sensitized photochemical solar cell system based on TiO(2) powders is very attractive from the point of view of potential low cost and high semiconductor photo stability. This project is an integrated program of basic and applied development research that is funded jointly by three U.S. Department of Energy program offices: the Division of Chemical Sciences in the Office of Basic Energy Sciences, the Photovoltaic program in the Office of Utility Technology and Advanced Energy Projects. In addition to the molecular dye-sensitized TiO(2) system, research is also occurring to study other organic heterojunctions with wide bandgap semiconductors for photovoltaic applications. The AEP portion of the project is to develop a configuration where the system is able to efficiently split water into hydrogen and oxygen, rather than to produce electricity. An inexpensive source of solar-produced hydrogen would be greatly beneficial to the energy economy of the world, and would result in the use of hydrogen as a non-polluting substitute for many of the fuels currently in use.

Naval Research Laboratory
Washington, DC 20375-5348

43. Silazymes--Rugged, High Capacity Enzyme-Mimetic Catalysts

Bruce Paul Gaber
Laboratory for Molecular Interfacial Interactions
202/404-6003

<u>Funding Profile</u>
Date Started: June 15, 1997
Anticipated Duration: 1 Year

FY 97 - $244,000

This project explores the novel wedding of two lines of biomolecular research- molecular imprinting and template directed materials synthesis. Methods will be explored to imprint the key components of an enzyme active site within the pores of an extremely stable, well-defined mesoporous silica matrix. If successful, the results of these investigations will lead to a new class of biocatalysts with an unprecedented combination of the versatility of enzymes and the stability of silica. The advantages of using enzymes for industrial scale chemical systems are manifold, including exceptional chemical specificity, high yield, simpler purification, novel reactions and reduction in waste solvents. Each advantage offers promise for energy savings in the bulk chemical industry- from synthetic costs to clean-up. Enzymes often cannot be applied to industrial processing because of an innate structural instability in extreme environments of temperature, non-aqueous solvents, and pH. The artificial enzymes being investigated in this work may provide a solution for the problems of enzyme fragility while maintaining all of the advantages of enzyme-based chemistry cited above. The mesoporous structure of the template implies high catalytic activity per unit volume, suggesting a cost-effective approach.

University of Nebraska
Lincoln, NE 68588-0111

44. Fabrication and Characterization of Micron Scale Ferromagnetic Features

Peter A. Dowben
Department of Physics
402/472-9838

Funding Profile
Date Started: July 15, 1995
Anticipated Duration: 4 Years*

FY 95 - $133,000
FY 96 - $101,000
FY 97 - $106,000

This is a project to study micro scale features of ferromagnetic nickel, cobalt, cobalt-palladium alloys and cobalt-palladium heterostructures fabricated by "direct writing," i.e. by selective area deposition from organometallic compounds. There are two goals for this research program. First, by making magnetic features smaller and smaller, in a variety of different shapes, the project will elucidate the influence of defects on magnetization reversal and coercivity. Second, the project will determine if there is any coupling between small ferromagnetic features (approx. 1 micron), possibly substrate mediated, on the length scale of 1000 angstroms smaller. This research project is based upon conventional methods for imaging magnetic domains. Polarized light microscopy permits not only imaging micron scale features but also determination of the magnetic orientation and coercivity with some spacial resolution. A microscope will be used to make polar Kerr rotation measurements and obtain spatially-selective magnetic information. A unique capability for probing the electronic structure of our magnetic features at resonance: spin polarized inverse photoemission with both longitudinal and transverse spin polarization will also be used. Essential to this project is a new technique for fabricating micro-scale ferromagnetic features. Organometallic chemical vapor deposition techniques sufficient to deposit pure metal features with excellent spacial resolution have been developed at this laboratory. These techniques allow selective deposition of large uniform arrays of nickel, cobalt, cobalt-palladium alloys and cobalt-palladium heterostructures in features as small as 0.2 microns, and as thin as a few monolayers or as thick as 10 microns. Multi layers can be made by the successive deposition of different metals or alloys by the sequential photolysis of different organometallic source compounds. While unconventional in many respects, this project utilizes a technology that is compatible with the fabrication of metal features 100 angstroms across in one Scanning-Tunneling microscopy run. The approach is superior to techniques employing ion beams or conventional lithography and is inexpensive and compatible with the fabrication of the next generation of optical and magnetic recording media.

*Includes 12 month no-cost extension

Oak Ridge National Laboratory
P.O. Box 2008
Oak Ridge, TN 37831

45. Biomolecular Optoelectronic Devices

Elias Greenbaum
423/574-6835

Funding Profile
Date Started: January 15, 1996
Anticipated Duration: 3 Years

FY 96 - $370,000
FY 97 - $350,000
FY 98 - $300,000

The purpose of this project is to accelerate the development of a practical device based on original Oak Ridge National Laboratory proof-of-principle scientific discoveries which were supported by the Division of Chemical Sciences, Office of Basic

Energy Sciences. It is motivated by knowledge of the intrinsic photophysical properties of the reaction centers of photosynthesis: nanometer dimensions, picosecond response times, and the ability to generate potential differences of about 1 volt upon absorption of a photon. This project is based on original discoveries in molecular electronics made at Oak Ridge National Laboratory. These include: 1) first demonstration of direct electrical contact with the electron transport chain of photosynthesis; 2) photoflash deposition of metallic platinum at the site of electron emergence from the Photosystem I reaction center of photosynthesis; 3) establishment of a novel platinization "welding" technique that allows construction of two-dimensional arrays of Photosystem I reaction centers on a metal surface; 4) first demonstration of a biomolecular diode in a single isolated photosynthetic reaction center; and 5) first demonstration of the compatibility of metallic platinum with the functionality of isolated Photosystem I reaction centers.

Oak Ridge National Laboratory
P.O. Box 2008
Oak Ridge, TN 37831-6085

46. Electrically Active Liquid Matrix Composites

Robert J. Lauf
Metals and Ceramics Division
423/574-5176

Funding Profile
Date Started: January 15, 1997
Anticipated Duration: 3 Years

FY 97 - $300,000
FY 98 - $300,000
FY 99 - $290,000

Varistors are nonlinear electrical resistors used to protect electrical equipment from the damaging effects of power surges. ZnO varistors are made by standard ceramic processes and are generally formed into cylinders or disks electroded on the end faces. Failure modes include catastrophic fracture, thermal runaway, and slow degradation of electrical properties. "Moldable" surge protective materials, comprising metal and semiconductor particles dispersed in a silicone rubber matrix, are not as nonlinear as ZnO but can be formed into a number of devices by injection molding. The material fails when an arc punches through at one point, leaving a carbonized, conductive path to ground. We have recently discovered that a slurry of metal, insulating, and semiconducting particles in dielectric oil can exhibit the same nonlinearity as the moldable rubber compositions, but with the added features that it is self-healing, thixotropic, and its I-V characteristics can serve as an excellent model system with which to study the poorly-understood electrical phenomena that occur in moldable varistors. In this project, we will: 1) determine the compositional limits for optimal electrical properties and relate these findings to theoretical percolation models; 2) determine the rheological properties of the experimental materials and identify promising avenues for improving them; and 3) determine the dielectric constants and the temperature dependence of key electrical properties.

Oak Ridge National Laboratory
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Oak Ridge, TN 37831

47. Shape Memory Alloy Reinforcement of Metals

Terry N. Tiegs
Metals and Ceramics Division
423/574-5173

Funding Profile
Date Started: December 15, 1996
Anticipated Duration: 3 Years

FY 97 - $405,000
FY 98 - $195,000
FY 99 - $290,000

A dispersed phase of shape memory alloy (SMA) has been employed to increase the hardness of a metal system. The hardness is well known to be directly related to the yield strength of the material and therefore a corresponding increase in the yield strength of the metal system is implied. The SMA works by generating an internal stress state in the matrix metal thereby increasing the stress required for yielding of the metal. The initial effort for the proof of principle used aluminum as the matrix material and NiTi for the shape memory alloy. The basic concept utilizes a dispersion of shape memory alloy particles in a metal matrix to induce internal stresses that increase the hardness and yield strength of the metal. The shape memory effect is a well known phenomenon observed in several material systems. Its characteristic are that when a SMA is mechanically deformed while below a specific transition temperature, it will return to its original shape, when the temperature is raised above the specific temperature. The shape memory alloy reinforcement of metals (SMART) works by: 1) taking a powder metallurgy-produced two-phase composite consisting of SMA particles dispersed in a metal matrix; 2) deforming the composite below the transition temperature; and 3) raising the temperature above the transition temperature to trigger the shape memory effect and induce internal stresses within the composite. Increasing the yield strength and hardness of materials is of considerable importance. Possible applications for SMART include high strength and lightweight structures for vehicles and industrial parts. Also these materials may be used for sensors and actuators where the reversibility of the shape memory effect could be utilized. To progress past the initial development stage for SMART, additional research and development is required. Such R&D would include development of optimum processing techniques, examination of the reinforcement-matrix interface, determination of the mechanical property envelope (including actual yield and ultimate tensile strength measurements) and survey the corrosion resistance of this class of composites.

Oak Ridge National Laboratory
P.O. Box 2008
Oak Ridge, TN 37831

48. Neutron Scattering and Polymer Synthesis in Environmentally Benign Supercritical Solvents

George D. Wignall
Solid State Division
423/574-5237

Funding Profile
Date Started: March 15, 1997
Anticipated Duration: 3 Years

FY 97 - $307,000
FY 98 - $278,000
FY 99 - $289,000

Above its critical point, carbon dioxide forms a supercritical fluid (SCF) which promises to be an environmentally responsible replacement for the organic solvents traditionally used in polymerizations. However, many challenges remain in implementing efficient synthetic strategies, as the reactions are thought to give rise to a wide range of submicron aggregates, but there has hitherto been no way to investigate such structures in situ. Over the past two decades, small-angle neutron scattering (SANS) has been developed as the premier characterization technique in this size range, and the penetrating power of the neutron beam means that SCF polymerization cells are virtually transparent. Polymers soluble in CO(2) include siloxanes and fluoropolymers, which have recently been characterized with respect to their molecular dimensions and thermodynamic interactions for the first time. Hydrocarbon polymers such as polystyrene (PS) are insoluble, though polymerizations may be accomplished via the use of PS-fluoropolymer stabilizers (soaps), which act as emulsifying agents. SANS has shown that these molecules form micelles with PS cores, which allow high polymerization yields. The development of CO(2)-based synthesis could reduce much of the wastes and emissions associated with current processes as the "CO(2)-solvent" could simply be recycled. Thus, no net CO(2) introduction to the atmosphere is entailed by this technology. We will address the many questions which remain to be answered concerning SCF polymerization mechanisms. The interactions between the polymer and surfactant give rise to a spectrum of particle morphologies and SANS has been widely applied to characterize similar structures in aqueous media. Thus, many of the outstanding issues in SCF polymerizations should be amenable to this methodology.

Ohio State University
Columbus, OH 43210-1106

49. Exploitation of Room Temperature Molecule/Polymer Magnets for Magnetic and Electromagnetic Interference Shielding and Electromagnetic Induction Applications

Arthur J. Epstein
Department of Physics
614/292-1133

Funding Profile
Date Started: July 15, 1996
Anticipated Duration: 3 Years

FY 96 - $322,000
FY 97 - $212,000
FY 98 - $215,000

There are increasing needs in today's society for lightweight, electromagnetic radiation shielding materials for operation at low frequencies (<MHz

range). This is partially driven by the growth of electric power distribution, telecommunications, and electromechanical power devices; concerns about electromagnetic interference; and an increasing need for lightweight inductive materials for efficient and portable motors and transformers. We reported the first polymer(tetracyanoethylene)-based magnet that remained strongly magnetic up to 350 K (170° F). We also demonstrated that more-than doubling of the room temperature magnetization can be achieved using a new route. Molecule/polymer-based magnetic materials are technologically attractive due to anticipated room temperature synthesis, processing, and device manufacture. Though these materials are relatively new, we already demonstrated that unoptimized versions of the materials shield magnetic fields independent of frequency between 10 and 10(4) Hz - a range difficult to shield using electrical conductors alone - with initial room-temperature real permeabilities of 13, which is close to iron. In late 1994, a preliminary report from a French group disclosed that a second class of molecule-based magnets (based on mixed-metal Prussian Blue type materials) has magnetic transitions near room temperature. The report suggests that additional molecule-based magnetic materials may be suitable for magnetic shielding. We have now synthesized similar (but not identical) Prussian Blue type materials with vanadium replacing iron. Our preliminary results on these modified Prussian Blue-type materials revealed an even higher saturation magnetization, though a lower transition temperature than reported by the French group, indicating opportunity for chemical tuning of the magnetic properties including initial permeabilities and transition temperatures. This project involves an integrated synthesis/processing/characterization/modeling component to ascertain the feasibility of using molecule-based magnetic materials, with emphasis on the study of the high Tc Prussian Blue-type magnetic materials, for shielding and induction applications from dc/low frequency to communications frequencies. The objective of this project is to establish the ultimately achievable intrinsic real and imaginary magnetic permeabilities and corresponding electric permittivities and their control through synthesis and processing.

Old Dominion University
Norfolk, VA 23529-0246

50. Micro-Hollow Cathode Discharge Arrays: High Pressure, Nonthermal Plasma Sources

Karl H. Schoenbach
Physical Electronics Research Institute
757/683-4625

Funding Profile
Date Started: July 15, 1996
Anticipated Duration: 3 Years

FY 96 - $229,000
FY 97 - $259,000
FY 98 - $210,000

Hollow cathode discharges are known as nonthermal plasma sources: the electron energy distribution in the two stages of the discharge (predischarge and main discharge) contains a large percentage of high energy (>10 eV) electrons. By reducing the size of the cathode holes from cm to ten's of microns, we were able to extend their range of operation from subtorr range to almost atmospheric pressure. The presence of high-energy electrons and the measured characteristics of micro-hollow cathode discharges, such as: 1) positive current voltage characteristics, which allow the construction of discharge arrays without ballast, 2) stable operation for dc, ac, and pulsed voltages, 3) low applied voltage (several hundred volts), and 4) strong radiative emission in the UV, allow the utilization of micro-hollow cathode discharge arrays (MHCDAs) for flat panel displays, surface processing, gaseous emission treatment, and as broad area electron and ion sources. The MHCDAs consist either of sets of metal meshes, spaced a distance on the order of the hole diameter apart, or of metal-plated, perforated dielectric foils. The simplicity, low cost, and the low required voltage for hollow electrode arrays makes MHCDAs strong competitors to other electro-technologies which rely on nonthermal plasmas (such as barrier discharges, and pulsed corona discharges). This project is studying the physics of micro-hollow cathode discharge operation in a positive differential conductivity mode. Particularly, the conditions for discharge array operation at atmospheric pressure are being explored, concentrating on the electron energy distribution and the spectral emission of micro-hollow cathode discharges. This project is focusing on two applications: 1) UV light sources (excimer lamps) for food and water sterilization and for surface treatment; and (2) gas reactors for treatment of hazardous gases, such as perfluoro compounds, used in the semiconductor industry, and volatile organic compounds (VOC's).

Pacific Northwest National Laboratory
Richland, WA 99352

51. Metal-Promoted and Semiconductor-Catalyzed Selective Alkane Oxidation

Donald M. Camaioni
Chemical Sciences Department
509/375-2739

Funding Profile
Date Started: January 15, 1997
Anticipated Duration: 4 years

FY 97 - $251,000
FY 98 - $337,000
FY 99 - $334,000
FY 00 - $104,000

The oxidation of hydrocarbons is of wide industrial and academic interest stemming from the importance of oxidation to the production of chemical feedstocks for numerous industrial processes. Enormous quantities of partially oxidized hydrocarbons (i.e., methanol, methyl tert. butyl ether, adipic acid, formaldehyde) are currently consumed by the public in the forms of transportation fuels, textiles, and resins. Industrial methods for their production suffer from tremendous energy inefficiencies. Researchers at the Pacific Northwest National Laboratory have discovered a potentially energy-efficient reaction sequence for selectively oxidizing saturated hydrocarbons, such as methane and cyclohexane, at ambient temperature and pressure. This reaction sequence is referred to as the ALKOX, or alkane oxidation, process and utilizes a Cu(I)/Cu(II)/O(2) system in acid media. This project will expand our understanding of ALKOX chemistry from its current conceptual stage to a point of pre-commercial viability. The research objectives are to: 1) obtain fundamental kinetic and mechanistic data on Cu(I)-promoted oxidation of methane and other hydrocarbons in acidic media; 2) obtain information about the identity of the oxidizing intermediate(s); (3) investigate modifications that may control oxidation selectivity; and 4) collect other data, such as mass balance, necessary to assess the commercial viability and applicability of the process. The results are expected to provide potential industrial clients the information they require to make licensing and investment decisions about the ALKOX process. Successful deployment of a direct, selective alkane oxidation process, such as the ALKOX process, can be used to exploit vast reserves of natural gas in the United States not currently being produced due to economics. This technology could also be used to produce more cost-effective oxygenated fuels and fuel additives and to lower the cost of producing oxygenated petrochemicals.

Princeton University
Princeton, NJ 08544-1009

52. Molecular Surface Modification as a Means of Corrosion Control

Andrew B. Bocarsly
Department of Chemistry
609/258-3888

Funding Profile
Date Started: June 15, 1996
Anticipated Duration: 3 Years

FY 96 - $388,000
FY 97 - $292,000
FY 98 - $309,000

Corrosion is a major materials problem in many industries. In the petrochemical industry which provides a major market for iron based materials, corrosion challenges exist from the production of hydrocarbons to their refining and conversion to chemical products. Corrosion of concern to the petrochemical industry occurs in a variety of environments ranging from highly acidic to alkaline, and temperatures ranging from room temperature up to ~1100° C. The goal of this research is to investigate the chemistry of novel organic films (corrosion inhibitors) of 5 angstroms to 20 angstroms dimension that may provide a corrosion resistant barrier on the surface of metallic materials. Joint studies at Princeton University and Exxon Research and Engineering Company suggest that developments in the fields of surface science and materials chemistry are now at a point where an utilitarian molecular view of corrosion processes is possible. This capability is expected to allow for the "molecular design" of next generation inhibitors having the requisite properties to provide for corrosion protection under extreme chemical and thermal conditions. In this project which is a collaborative effort involving members of the Princeton Materials Institute and scientists from Exxon's Research and Engineering Laboratory, state-of-the-art surface characterization tools will be brought together to generate a molecular level understanding of model organic films appropriate for corrosion control. The mechanisms of film protection and film breakdown will be investigated thoroughly. The order and packing density of the films will be studied as a function of temperature, using Grazing Incidence X-ray Diffraction involving synchrotron X-radiation as a main characterization tool. The interface stability of the molecule, its bonding mechanism and dissociation pathways will be studied by using a combination of spectroscopies such as Temperature Programmed Desorption, High Resolution Electron Energy Loss Spectroscopy and Auger Electron Spectroscopy on model substrate surfaces. Additionally, low energy electron diffraction will be used to characterize the material surface after molecular debonding. The mechanistic understanding derived from these different techniques will be used to construct molecular frameworks that may provide corrosion resistance. The performance of these molecular architectures in real environments will be investigated using electrochemical reactors available at Exxon's Corporate Research Laboratories.

Princeton University
Princeton, NJ 08544-1009

53. Optimally Controlled Interior Manipulation of Solids

Herschel Rabitz
Department of Chemistry
609/258-3917

Funding Profile
Date Started: November 19, 1992
Anticipated Duration: 4 Years (Project Completed)*

FY 93 - $329,000
FY 94 - $349,000
FY 95 - $299,000

In the processing of solid state materials, manipulation or modification is usually confined to their accessible exterior surfaces. This project is concerned with the development of a technique for modification of the interior solids without the necessity of opening up the material. The technique is based on the concept of designing and creating temporally and spatially tailored laser pulses that deposit energy on the surface for the purpose of launching an intense acoustic wave that focuses within the solid. Taking account of the relatively large illumination area on the surface and the focusing nature of the acoustic waves, it should be possible to minimally disrupt the surface while still attaining significant degrees of interior modification at the target volume. A central feature of this new materials processing method is its reliance on destructive and constructive interference between the ensuing shear and compressional acoustic waves. The delicacy of this method calls for the use of optimal design and control techniques for the temporal and spatial shaping of the laser beams. The research will consist of a theoretical design effort that closely interacts with a laboratory program for implementation of the design concepts. The research will be conducted in a series of steps, starting with low intensity focusing and proceeding to the regime where permanent solid interior alteration is possible. In accord with this sequential development, theoretical design work will move from the linear to the nonlinear regimes of solid mechanics and the laboratory studies will involve increasing laser pulse intensities and complexities of pulse shapes. The overall purpose of the research is to establish the feasibility of achieving interior manipulation of solids. Particular attention will be paid to discerning the flexibility as well as limitations of the physical process. An established capability for interior manipulation of solids would open up many opportunities including interior annealing, induced phase transitions, induced chemical reactions, crack arresting, controlled defect site generation, and interior welding.

*Includes 12 month no-cost extension

University of Richmond*
Richmond, VA 23173

54. Association of N(2)-Fixing Cyanobacteria and Plants: Towards Novel Symbioses of Agricultural Importance

Jeff Elhai
Department of Biology
804/289-8412

Funding Profile
Date Started: September 1, 1997
Anticipated Duration: 31 Months**

FY 97 - $157,000
FY 98 - $201,000

The ever growing demand for nitrogenous fertilizers with their attendant energy cost and environmental complications, makes the alternative of biological N(2)-fixation increasingly attractive. Cyanobacteria comprise a significant portion of all N(2)-fixing microorganisms. Many can form symbiotic associations with diverse plants and fungi, but no case is known of a productive association of a cyanobacterium with an agriculturally important plant. Recently, we have demonstrated the ability of certain cyanobacteria to form intimate associations with wheat and rice and to penetrate the tissue of these plants. We will extend this work by addressing the following questions: 1) What is the most efficient method of introducing cyanobacteria into wheat? 2) What is the fate, location, and metabolic activity of cyanobacteria upon introduction into plants? 3) What is the cyanobacterial contribution to the nitrogen budget of the plant? And 4) What is the range of plants capable of forming such association? The fate and metabolic activity of cyanobacteria incorporated into plants will be monitored by a novel DNA-based method we have developed and by using cyanobacteria genetically tagged with genes encoding luciferase, an enzyme that produces luminescence. Different techniques of introducing cyanobacteria into plants, such as penetration via root, via stomata, co-culture of plant calli with cyanobacteria, and creation of nodule-like structures of plants and their colonization with cyanobacteria, will be considered. Cyanobacterial contribution to plant nutrition will be determined by measuring plant nitrogen content and (15)N incorporation. The results of these experiments may provide insight as to the requirements for exploiting N(2)-fixing cyanobacteria in the field and the benefits that may be expected.

*This project was started on April 1, 1996, at Florida International University.

**Includes 2 month no-cost extension. The total three-year funding for this project is $520,000.

Sandia National Laboratories
Albuquerque, NM 87185-0346

55. Semiconductor Broadband Light Emitters

Paul Gourley
505/844-5806

Funding Profile
Date Started: December 1, 1994
Anticipated Duration: 3 Years

FY 95 - $330,000
FY 96 - $382,000
FY 97 - $390,000

Semiconductors are compact, lightweight, operate in air, and are rugged. However, conventional semiconductor diodes emit light only in a narrow range of wavelengths. To obtain broadband emission, new structures are needed that utilize a wide range of alloy compositions available from modern semiconductor growth techniques. Fractal lattice and chirped quantum wells form a new class of materials which can provide broadband light emitters. The goal of this project is to develop such multi-alloy structures grown by metal organic vapor phase epitaxy and molecular beam epitaxy for efficient, broadband light emission. To develop broadband emitters, we will focus our efforts on this class of fractal and chirped quantum-well structures utilizing InAlGaP alloys grown by metal-organic vapor phase epitaxy on GaAs substrates. The work will concentrate on three areas: materials design and growth, characterization and modeling, and device design and fabrication. The interplay of these three parallel efforts will lead to optimized device structures that emit broadband light with at least 300 meV bandwidth in the green to red regions and a few percent external quantum efficiency. Materials and design parameters will be understood through a wide variety of experimental and theoretical tools. To implement this new class of broadband emitters, we will design, grow and fabricate light-emitting diode structures, and measure electro luminescence spectra, current-voltage, and light-current characteristics.

Sandia National Laboratories
Albuquerque, NM 87185-0346

56. Rapid Melt and Resolidification of Surface Layers Using Intense, Pulsed Ion Beams

Bob Turman
505/845-7119

Funding Profile
Date Started: November 1, 1994
Anticipated Duration: 3 Years

FY 95 - $300,000
FY 96 - $300,000
FY 97 - $300,000

In the past, the introduction of new material surface treatments like galvanizing, sputtering, and plasma spraying have enabled new products and opened new markets. The capability to rapidly melt and resolidify surface layers using intense, pulsed ion beams can enable another such advance. This project will develop a next-generation surface processing technology based on new, repetitively-pulsed ion beams. Rapid solidification is known to greatly improve metal surface properties such as corrosion, wear, and fatigue resistance, but the lack of an economic and effective way to apply this technique to surfaces has prevented its use except in high value applications. Intense, pulsed, high energy ion beams treat surfaces through surface melting followed by rapid thermal quenching by thermal diffusion into the underlying, untreated bulk material. This process produces non-equilibrium micro-structures, nanocrystalline phases, and extended solid solutions leading to improved corrosion and friction properties of metals, as well as surface smoothing and defect healing, grain refinement, and modification of surface layer hardness. The low cost and in-depth deposition of high energy pulsed ion beams gives pulsed ion beam technology important advantages over laser treatment. The project will determine the capabilities and limitations of rapid melt and resolidification using pulsed ion beams. It will document the non-equilibrium micro-structures produced in treated layers and their effect on metal surface properties and will do the initial process development needed to show how this technique can be applied to commonly used metals. If successful, this will enable new ways to modify surfaces for enhanced properties and lifetimes with greatly improved energy efficiency and cost-effectiveness and will enable a significant reduction in the use of heavy metal and solvent-based surface treatment coating processes.

University of South Florida
4202 E. Fowler Avenue
Tampa, FL 33620-5700

57. Experimental and Theoretical Investigation of Dual-Laser Ablation for Stoichiometric Large-Area Multicomponent Film Growth

Sarath Witanachchi
Department of Physics
813/974-2789

Funding Profile
Date Started: August 15, 1996
Anticipated Duration: 4 Years*

FY 96 - $147,000
FY 97 - $108,000
FY 98 - $113,000

We have recently discovered a novel dual-laser ablation process that dramatically alters the dynamics of the conventional single-laser ablation process. Initial experiments, using this process, allowed the production of high quality, defect-free films of $Y(2)O(3)$ that were not possible with single excimer laser ablation. This provided the motivation for investigating the physical mechanisms operative in this novel process. Two major problems associated with single laser ablation have hindered the development of this method as a manufacturing process. They are: 1) deposition of micron and submicron particulates; and 2) relatively narrow expansion profiles that limit the area of uniform film growth. Dual-laser ablation can potentially overcome both these major drawbacks while retaining the main advantages of the single laser ablation technique. A systematic study will be used to ascertain expansion characteristics of individual elements, with different volatility, in a multi-component material system, under the dual-laser ablation process that would determine the required conditions for large-area defect-free stoichiometric film growth. A species-sensitive hydrodynamic model will be used. This will provide a clear understanding of the basic mechanisms operative in this process, and thus aid the process optimization for any material system. The dual-laser ablation system comprises a tandem combination of excimer and $CO(2)$ laser pulses with an adjustable inter-pulse delay, that is spatially overlapped on the target. The primary objective of the research is to study experimentally the effect of the process parameters on the species velocity distribution and expansion profile for individual components, and to develop a species-sensitive theoretical model that is consistent with the experimental observations. The project will investigate a Cu target to establish the process characteristics for a single-element plume. It will also study the expansion characteristics of CuInSe(2) and Cu(In(1-x)Ga(x))Se(2) plumes to explore the behavior of individual elements in multi-component plumes. Investigation of spatial stoichiometric control of Ga in the Cu(In(1-x)Ga(x))Se(2) will aid semiconductor doping studies. The new understanding of the dual-laser ablation process will facilitate the extension of this method to other material systems. The method offers ease of control, simplicity and high-quality film growth, that could yield a method of choice for both epitaxial and highly oriented polycrystalline multi-component film growth.

*Includes 12 month no-cost extension

TecOne
1803 Sageway Drive
Tallahassee, FL 32303

58. 'Off-Diagonal' Thermoelectricity for Cooling and Power Generation

Louis R. Testardi
904/562-9789

Funding Profile
Date Started: June 1, 1995
Anticipated Duration: 2 Years (Project Completed)

FY 95 - $170,000
FY 96 - $166,000

'Off-Diagonal' thermoelectricity, an uncommon effect which only occurs in low symmetry materials, allows unique and untried opportunities for thermal cooling, heat pumping and power generation. It utilizes the orthogonal coupling of heat and electric current flows in anisotropic media and opens new device as well as material development routes for the improvement of thermoelectric energy conversion. The advantages lie in a geometry naturally adapted to compact cooling, heat pumping and power generation with planar thermal boundaries, and also in electric impedances which allow a more compact, efficient and convenient device. The overall project goal is the development of a lightweight, flexible sheet material which will provide cooling, heat pumping and, with less application, power generation for objects or temperature baths of irregular geometry using 'off-diagonal' thermoelectricity. The principal materials thrust will be in conducting polymers because of their potential low cost and their ease of large scale processing to develop anisotropic properties. Applications include cooling of small volume consumer/industrial items, cooling and temperature control of the human body for medical treatment and comfort, and the utilization of waste heat from large area temperature baths.

Texas A&M University
College Station, TX 77843

59. Layer-by-layer Growth of Organic Thin Films in the Absence of Solvents

Richard M. Crooks
Department of Chemistry
409/845-5629

Funding Profile
Date Started: June 15, 1997
Anticipated Duration: 3 Years

FY 97 - $155,000
FY 98 - $ 79,000
FY 99 - $ 80,000

The objective of this project is to develop the chemistry necessary to construct oriented, organic thin films on surfaces by direct reaction at the solid-vapor interface in the absence of solvents. The reactants and the reaction by-products are entrained in nitrogen gas or in supercritical carbon dioxide. In general, it appears that many types of chemical reactions are amenable to solvent-free reaction conditions as long as the reactants and the by-products have sufficient vapor pressure and the reaction does not require the use of catalysts. Although these constraints limit the versatility of the proposed approach somewhat, they are balanced by some fundamentally and technologically important advantages: 1) the need for solvents and solvent disposal is eliminated; 2) undesirable solvent effects on the thin-film structure and the reaction chemistry are eliminated; 3) reaction chemistry on high-energy organic surfaces can be carried out in the absence of solvent-phase impurities; 4) mass transfer and reaction rates are often much higher in vapor phase ambients than in solution; 5) certain types of useful chemistry, such as hydrogen bonding, are enhanced at the vapor/solid phase interface; and 6) vapor phase reaction chemistry lends itself to automation and commercialization. While elucidation of the chemistry necessary to fabricate such films is interesting in itself, the structures proposed for study will find use in a wide range of technologically and commercially important applications including those related to lithography, corrosion inhibition, friction, lubrication, adhesion, chemical sensing and non-linear optics.

Texas A&M University
College Station, TX 77843

60. Utilizing Laser Spectroscopy of Noble Gas Tracers for Mapping Oil and Gas Deposits

Hans A. Schuessler
Physics Department
409/845-5455

Funding Profile
Date Started: December 15, 1992
Anticipated Duration: 5 Years*

FY 93 - $152,000
FY 94 - $164,000
FY 95 - $168,000

Radioactive noble gases are being used as tracers to measure the structure of gas and oil deposits. Due to their chemical inertness, they offer the advantage that they do not react with the environment with which they are in contact. Usually, a noble gas tracer is injected at an injection well and gas or liquid samples are taken from a production well. When a long-lived tracer, such as (35)Kr (half-life = 10.8 y), is used for extended deposits, the specific activities of the production well samples are low. The measurements are then difficult, since the sample must be analyzed in an ultra low counting facility to minimize the background counts. This problem exists even when large amounts of tracer gas with high radioactivity levels (several hundred curie) are injected for which extensive safeguarding of the personnel is necessary. The objective of this project is to improve the sensitivity of noble gas detection in samples taken from production wells by more than three orders of magnitude by applying optical rather than nuclear detection. The novel technique will not only reduce the required radioactivity levels at the injection site, but work even with stable tracer isotopes thus abolishing most handling, transportation and storage problems. Collinear fast beam laser spectroscopy will be used for which a sensitivity at the few atoms level and also complete isotopic selectivity has already been demonstrated. The construction of a prototype analytical instrument is planned that can routinely and quickly analyze samples for their noble gas content. Single noble gas atoms can then be detected, even in the presence of other isotopes and atoms which are more abundant by a factor of about 10(15). Since sample enrichment might not be necessary and stable noble gas tracers are inexpensive, the method promises to be more cost effective and environmentally safe than present nuclear decay detection.

*Includes 24 month no-cost extension

University of Texas
Odessa, TX 79762-8301

61. A Mild, Chemical Conversion of Cellulose to Hexane and Other Hydrocarbon Fuels.

J. Michael Robinson
Chemistry Department
915/552-2237

Funding Profile
Date Started: January 15, 1995
Anticipated Duration: 41 Months*

FY 95 - $350,000
FY 96 - $300,000
FY 97 - $260,000

This project will develop a mild chemical reduction process that converts biomass with 100% carbon conversion into a hydrocarbon fuel. There are five requirements for such a conversion. 1) The carbon chain remains intact. 2) Each reaction occurs at mild conditions and gives a high yield. 3) Each reaction is catalytic and only hydrogen or electricity is consumed. 4) Initial reactions occur in an aqueous medium, which 5) allows the use of wet feedstocks. These requirements will be addressed beginning with the continued exploration of unique chemical reductions of components derived from biomass. Catalytic recycling of the chemical reducing agents provides the equivalent of an efficient biomass reduction. The objective of this project is to develop an efficient multi step chemical process for the conversion of the principal components of biomass, cellulose and hemicellulose, into hydrocarbon fuels. Separation of biomass into individual components allows use of selective reactions that give 100% carbon conversion. With a multi step reaction design, a single pure product such as hexane may result instead of a crude fuel mixture which results from pyrolysis methods.

*Includes 5 month no-cost extension

Tufts University
4 Colby Street
Medford, MA 02155

62. A Sodium Cycle Based Organism With Improved Membrane Resistance Aimed at Increasing the Efficiency of Energy Biotransformations

Kim Lewis
Biotechnology Center
617/627-3251

Funding Profile
Date Started: July 15, 1997
Anticipated Duration: 3 Years

FY 97 - $124,000
FY 98 - $127,000
FY 99 - $133,000

Oxidative phosphorylation based on a H+ cycle creates the problem of membrane proton leaks that inevitably arise in the presence of organic solvents and alcohols employed in energy bioprocessing technologies. A radical solution to this problem is to replace the conventional H+-cycle mechanism of oxidative phosphorylation with an Na+-cycle, creating an organism that will have a significantly higher resistance to membrane-acting agents. Such an organism will be of considerable value for many biotechnological applications. For example, desulfurization of low-grade oil by bacteria is carried out in environments that are toxic to the cell. The H+ leak leads to a collapse of the proton motive force, which is the intermediate linking oxidation of substrates to ATP synthesis. The membrane is 100- to 1000-fold more resistant to leaks of a larger Na+ ion. An organism with Na+ substituting for H+ in energy transductions will therefore produce a cell with a considerably higher resistance to agents affecting the membrane. This is a high-risk, high-return proposition. What makes this project attractive is the fact that all the blocks for building a sodium cycle exist in nature. The genes that code for the Na+-pumping respiratory chain of marine *Vibrio alginolyticus* and fresh-water aerobe *Vitreoscilla*, will be combined with the Na+-dependent ATPsynthase of the marine anaerobe *Propionigenium modestum* in one organism. A portable gene kit for Na+-based oxidative phosphorylation will be assembled, using E.*coli* as a host. The project will progress in stages, starting with expressing functionally a single primary Na+-pump in E.*coli*, the Na+-NADH dehydrogenase. A sodium ATPsynthase will then be added, creating a minimal complete sodium cycle. This first-generation organism will have mixed H+-and Na+-cycle oxidative phosphorylations. The project will progress in the direction of gradually replacing the elements of the H+ cycle with genes coding Na+-cycle. Resistance of the engineered organisms to both specific protonophores and non-specific toxic agents such as organic solvents will be studied. Once the minimal gene kit for the Na+-cycle is assembled in E.*coli*, we will clone it into *Rhodococcus*, an organism utilized in oil desulfurization. A possible increase in the efficiency of oil sulfurization will be tested by our collaborators from Energy BioSystems Corporation.

University of Washington
Seattle, WA 98195

63. Cryogenic Energy Storage System for Automotive Propulsion

Abraham Hertzberg
Aerospace and Energetics Research Program
206/543-6321

Funding Profile
Date Started: June 1, 1995
Anticipated Duration: 3 Years*

FY 95 - $175,000
FY 96 - $186,000

Studies at the University of Washington indicate that liquid nitrogen is an effective energy storage medium which, when used for automotive purposes, offers significant advantages over current and proposed battery systems, both in performance and economy. Reasonably-sized liquid nitrogen propulsive systems can provide automotive ranges between 200 and 300 miles, with operating costs well below those of any other electric vehicle concept. The range and performance can readily be extended with the addition of a small, low temperature combustor when operating as an ultra low emission vehicle. Some of the particular advantages are that refueling the cryogen only requires minutes and there are not environmental hazards in introducing a liquid nitrogen energy storage infrastructure. This project is designed to explore the advantages of a liquid nitrogen energy storage system for automotive propulsion. In the first year the work will concentrate primarily on the heat exchanger element. During the second year a prototype heat exchanger system will be fabricated and tested under simulated road conditions.

*Includes 12 month no-cost extension

University of Washington
Seattle, WA 98195

64. The Supersonic-Mixing, Shock-Wave Reactor: An Innovative Approach for Efficient Chemical Production

Arthur T. Mattick
Aerospace and Energetics Research Program
206/543-6181

Funding Profile
Date Started: June 15, 1993
Anticipated Duration: 4 Years (Project Completed)*

FY 93 - $272,000
FY 94 - $418,000
FY 95 - $309,000

The production of many commercially-important chemicals involves pyrolysis of hydrocarbon feedstocks, an energy-intensive process that is now carried out by heating components of oil or natural gas in a furnace. This research will examine the potential of a novel approach for pyrolysis, the supersonic-mixing, shock-wave reactor, for reducing the energy consumption and production cost of ethylene and other compounds. These benefits arise from the use of gas dynamic processes to precisely control the temperature history of a reactant and thereby maximize the yields of valuable products. Initial studies indicate that ethylene yields in the pyrolysis of ethane may be 20-40% higher by using this method in place of conventional technology, and energy consumption may be reduced by 15% or more. This research project entails: 1) experimental investigation of fundamental aspects of supersonic mixing and reacting gas streams, such as mixing shear layers, shock structure and uniformity, and reaction pathways, that are important in the reactor's operation; 2) measurement of product yields under conditions of pyrolysis expected in commercial applications of the reactor; and 3) examination of methods of implementing the reactor for chemical manufacture.

*Includes 12 month no-cost extension

Western Washington University
Vehicle Research Institute
Bellingham, WA 98225-9086

65. A Thermo-Photovoltaic Generator for Use in a Lightweight Electric Car

Michael R. Seal
Department of Technology Engineering
360/650-3045

Funding Profile
Date Started: August 1, 1994
Anticipated Duration: 38 Months
(Project Completed)

FY 94 - $145,991
FY 95 - $444,871
FY 96 - $299,851

In an internal combustion engine, fuel is mixed with air and exploded. Because the explosions are of very short duration, the combustion is incomplete, leading to carbon monoxide and hydrocarbon exhaust emissions. More pollution results because the temperature at the peak of the explosion is very high leading to the creation of nitrous oxides. A quiet, lightweight, clean, electric power source will be built in which a fuel is continuously burned in a ceramic tube, the tube glows red hot, and photovoltaic cells receive the infrared from this emitter and convert it to electric power. In effect, "solar" cells are used with a small manmade "sun" created by burning natural gas. Because fuel is burned continuously without periodic explosions, the thermophotovoltaic unit is very clean, quiet, efficient, and lightweight. The first bench top experiments have already shown that this generator is 50 times cleaner than an internal combustion engine. Such a thermophotovoltaic unit has only recently become feasible as a result of new gallium antimonide cells fabricated by the JX Crystals Company. These new cells are much more sensitive in the infrared range than traditional solar cells. These new infrared cells will be integrated with an efficient natural gas fired infrared source with sufficient power to charge onboard vehicle batteries. The thermophotovoltaic eight cylinder unit alone will be able to maintain an automobile at a speed of 60 miles per hour on level ground. Additional power for hill climbing and performance will be provided by onboard batteries.

*Includes 2 month no-cost extension

Yale University
New Haven, CT 06520-8120

66. Cyclotron Autoresonance Accelerator for Electron Beam Dry Scrubbing of Flue Gases

Jay L. Hirshfield
Physics Department
203/432-5428

Funding Profile
Date Started: April 1, 1997
Anticipated Duration: 3 Years

FY 97 - $293,000
FY 98 - $310,000
FY 99 - $295,000

The objectives of this project are to design, construct and evaluate a novel rf electron accelerator for electron beam dry scrubbing (EBDS) of flue gases emanating from fossil-fuel burners. This machine, a cyclotron autoresonance accelerator (CARA), has already shown itself capable of converting rf power to electron beam power with efficiency values as high as 97%. This *efficiency level is higher than that for existing rf* industrial linear accelerators and helps to sustain the economic argument in favor of EBDS, in comparison with conventional methods of flue gas scrubbing. Early in the three-year research effort, designs will be developed for high efficiency production of 1.0 MeV, 33 megawatt electron beam pulses based on use of up to 24 MW of rf power at 2.856 Ghz available at Yale. Construction of this accelerator will involve installation on Yale's existing gun modulator. Evaluations of the self-scanning beam from the high-power CARA for EBDS applications will involve extraction of the beam through an appropriate window and measurement of the radiation dose delivered to a gas cell and beam dump. Designs and cost estimates will be formulated for a 100 kW average power CARA that could in the future be used in an EBDS demonstration pilot plant. In addition to application in EBDS, other versions of high-power CARA's could find use in treatment of waste sludges, sterilization of medical supplies and foodstuffs, in sources of high power microwaves, and as a high power rf-to-dc rectifier for power beaming.

SMALL BUSINESS INNOVATION RESEARCH (SBIR) PROGRAM
AND
SMALL BUSINESS TECHNOLOGY TRANSFER (STTR) PROGRAM

SBIR

The Small Business Innovation Research (SBIR) program was created in 1982 by Public Law 97-219 and reauthorized in 1992 until the year 2000 by Public Law 102-564. Program objectives are: to increase private sector commercialization of technology developed through Federal R&D; to increase small business participation in Federal R&D; and to improve the Federal Government's dissemination of information to women-owned-, and economically-disadvantaged small business concerns.

Agencies with extramural R&D budgets of over $100 million are required to conduct an SBIR program using a set-aside of a stated percentage of that budget. The percentage increased from an initial 0.2% in 1983 to 1.25% in 1986 through 1992. Public Law 102-564 increased the set-aside further, starting with 1.5% in 1993 and reaching a maximum of 2.5% in 1997. The Department's SBIR budget for FY 1997 was about $74 million.

In the Department of Energy, SBIR funds are used to support an annual competition for Phase I awards of up to $75,000 for about 6 months to explore the feasibility of innovative concepts. Only Phase I winners are eligible to compete for Phase II, which is the principal research or R&D phase. The maximum funding for Phase II projects in FY 1997 is $750,000 over a two-year period. Technical topics for DOE's annual SBIR Solicitation are compiled by program managers in the agency.

In Fiscal Year 1997, the Advanced Energy Projects Division (AEP) is managing four Phase II SBIR projects selected from grant applications submitted to the topic, "Novel Materials for Sustainable Energy Development," in the 1995 DOE SBIR Program Solicitation. All are from the subtopic "Novel Materials for Direct Energy Applications or Replacement Products or Components." In addition, AEP is managing two Phase II SBIR projects selected from applications to the topic "Mechanical Miniaturization and Nanoscale Electronics for Energy Applications," in the 1996 SBIR Program Solicitation, one from the "Submicron-Scale Electronic Materials" subtopic and the other from the "Micromotors and Micromechanical Instruments" subtopic.

STTR

The Small Business Technology Transfer (STTR) program was established under Title II of the Small Business Research and Development Enhancement Act of 1992, Public Law 102-564. Under this program, funds are reserved for awards to small businesses for cooperative R&D to be conducted jointly with a nonprofit research institution. The set-aside of the extramural R&D budget used to fund this program is 0.05% in FY 1994, 0.10% in FY 1995, and 0.15% in FY 1996 and 1997. The DOE STTR budget was about $4.6 million in FY 1997.

STTR is similar to SBIR in that the primary goal of both programs is to increase private sector commercialization of technology developed through Federal R&D. Unique to STTR is the requirement that 40% of the work must be performed by the small business and at least 30% of the work must be performed by the non-profit research institution. Such institutions include Federally-funded R&D centers, DOE national laboratories, universities, and other non-profits.

In Fiscal Year 1997, AEP managed three Phase I STTR projects awarded under the topic "Novel Materials for Energy Applications."

PHASE II SBIR PROJECTS

Aspen Systems, Inc.
184 Cedar Hill Street
Marlborough, MA 01752-3017

67. Low Cost, Contamination-Tolerant Electro catalysts for Low-Temperature Fuel Cells

Jaeseok Ryu
508/481-5058

Funding Profile
Date Started: July 9, 1996

FY 96 - $343,750
FY 97 - $406,250

Power generation from fuel cells via reformed gaseous fuel or direct methanol oxidation is a very attractive option for fuel cell vehicles or other mobile systems. One of the major road blocks to large-scale consumer applications of the fuel cell technology is the high cost and limited supply of the noble metal-based catalysts and catalyst poisoning. Group VI metal carbides, such as molybdenum carbides, tungsten carbides, or their mixtures, exhibited high catalytic activity toward electro-oxidation of the methanol. In addition, these catalysts are tolerant of CO contamination in the reaction zone. In order to develop low cost, contamination-tolerant Electro catalysts, Aspen Systems proposes an innovative chemical reduction process. In Phase I, we successfully produced nanosize metal carbides via a chemical reduction process. Measured crystallite size of metal carbides was as small as 2.5 nm. We also demonstrated relatively good electro catalytic activity of the metal carbides for hydrogen oxidation, oxygen reduction and direct methanol oxidation. In addition, we experimentally demonstrated the CO-tolerant nature of metal carbides. Electrochemical performance of these catalysts were not affected by 100 ppm CO concentration in hydrogen. In Phase II, we will optimize the chemical reduction process and post-heat treatment conditions to further improve electrochemical activity of these materials. We will also optimize the electrode structure/configuration to fully utilize the fine particle size of these catalysts. In addition, we will fabricate membrane electrode assemblies; utilizing metal carbide catalysts. Finally, we will demonstrate the contaminant-tolerance of the single cell with metal carbide catalysts by operating it on CO-containing hydrogen (up to several % CO).

Giner, Inc.
14 Spring Street
Waltham, MA 02154-4497

68. An Integrated Catalyst/Collector Structure for Regenerative Proton-Exchange Membrane Fuel Cells

Larry L. Swette
617/899-7270

Funding Profile
Date Started: July 9, 1996

FY 96 - $379,597
FY 97 - $339,550

Dedicated proton-exchange membrane (PEM) fuel cells, electrolyzers and single-unit regenerative fuel cells (RFCs) have been identified by DOE as simplified technology of potential benefit to the electric vehicle and energy storage programs. Bifunctional catalysts and electrode structures to support the alternating gas evolution/consumption modes of PEMRFCs have been developed by Giner, Inc. for both negative and positive electrodes. Full implementation of this technology requires the development of a suitable gas-diffusion/current-collection interface (GCI) structure for the positive electrode to yield superior performance, stability and simplicity in bifunctional operation. The GCI structure proposed for development is based on a stabilized, wetproofed porous metal sinter with embedded shapes on the gas side (channels or pin fields) to facilitate bulk fluid distribution, and a flat surface on the membrane side to which a thin catalytic layer can be laminated. In Phase I, the potential feasibility of several small size prototype approximations of this GCI structure were evaluated. Three types of porous metal sheet were successfully prepared (two with machined grooves), stabilized, wetproofed, catalyzed and tested in a small PEMRFC (36 cm^2), with promising results. For Phase II we propose the development of integral embedded shapes in the porous metal sinter together with some variations in porosity and pore size. When suitable structures have been identified they will be scaled up (e.g., 5"x 5", 160 cm^2) and tested more extensively as both single cells and multi-cell stacks.

Harvest Technology
9253 Glen Oaks Boulevard
Sun Valley, CA 91352-2614

69. Molten Film High-Intensity Paper Drying

David Warren
818/767-3157

Funding Profile
Date Started: July 9, 1996

FY 96 - $326,834
FY 97 - $363,059

A novel, molten-fluid drying technology is being developed to substantially reduce the capital and operating costs for the manufacture of paper products such as writing papers, packaging papers, and paperboard. The technology involves contacting molten fluids of unique property against the wet paper web so as to impart heat for drying in a more energy efficient and cost effective manner compared to current evaporative dryers. Phase I tests using prewetted commercial kraft papers of 30# and 75# grade were conducted on an experimental molten fluid dryer which showed that average drying rates of 40 lb/ft(2)/hr, or an order of magnitude higher than current cylinder drying technology, were achievable without the use of ventilation air. Engineering studies indicate that the dryer can reduce equipment size by 60%-75% and capital costs by greater than 50%. Because no ventilation air is required, the dryer energy efficiency is increased by 20% and the recoverable waste heat dramatically increases from 10% to 90%. SEM/EDX analyses showed that no molten material adheres to the paper surface during drying, and product property measurements showed the dried paper samples to be of high quality. The Phase II program will involve construction and testing of a molten fluid drying system with a drying capacity of 1000 lb/hr of sheet moisture. After initial development and testing, the dryer will be integrated with a Black Clawson pilot-scale paper machine to assess the performance of this technology under conditions that closely simulate the commercial production environment. These tests will provide the basis for Phase III field demonstration tests at an operating mill.

Integrated Microtransducer Electronics Corp.
1214 Oxford Street
Berkeley, CA 94709-1423

70. Nanoscale All-Metal Electronics

Richard Spitzer
510/841-3585

Funding Profile
Date Started: June 18, 1997

FY 97 - $371,914
FY 98 - $371,916

Improvements in the performance and price of semiconductor integrated circuits have been accompanied by a sharp rise in capitalization costs. Additionally, semiconductor devices are vulnerable to radiation and their miniaturization is limited because of charge leakage. An all-metal electronics technology offers the promise of better energy efficiency and substantially lower manufacturing costs than those of silicon integrated circuits. This project examines new technology that uses giant magnetoresistance (GMR) films rather than semiconductors to make electronic components and other devices. During Phase I, thin film micron-scale transformers using GMR films were designed and fabricated. Phase II will design, fabricate, and test various logic circuits using GMR transistors and transformers. Additionally, the GMR components will be optimized.

Nanomaterials Research Corporation
2849 East Elvira Road
Tucson, AZ 85706-7126

71. Passive Electronic Components From Nanostructured Materials

Thomas Venable
520/294-7115

Funding Profile
Date Started: June 18, 1997

FY 97 - $390,625
FY 98 - $359,375

Passive electronic components play a critical role in ensuring efficient and reliable generation, delivery, and use of energy. Existing passive components were discovered a few decades ago and are all based on bulk material properties. Although miniaturization of these components have enabled dramatic performance improvements, it is anticipated that fundamental breakthroughs would be necessary to satisfy future needs of electrical, electronics, and energy systems. Nanostructured materials - materials whose domain sizes have been confined to dimensions less than 100 nm - potentially offer such a breakthrough because of the unique combination of non-bulk like properties they exhibit. During Phase I, significantly superior passive electronic components were prepared from nanostructured materials and their performance was demonstrated. Phase II will optimize nanomaterials device manufacturing and performance, build prototypes, field test the prototypes, and initiate commercialization.

Nanomaterials Research Corporation
2849 East Elvira Road
Tucson, AZ 85706-7126

72. Nanostructured Interstitial Alloys as Catalysts for Direct Energy Applications

Tapesh Yadav
520/294-7115

Funding Profile
Date Started: March 24, 1996

FY 96 - $361,826
FY 97 - $388,174

According to some estimates, U.S. manufactured products that depend on catalysis technologies account for over $500 billion per year and include petroleum products, vehicle and industry emission controls, chemicals, pharmaceuticals, plastics and rubber, and food products. But frequently, precious metals such as platinum (Pt) and palladium (Pd) must be used as catalysts. They have the disadvantage of being expensive ($3,000 to $15,000/lb) and must be imported in large quantities. A breakthrough in catalyst performance and catalytic materials could enhance U. S. competitiveness, reduce environmental impact, and improve energy efficiencies. During Phase I, a proof-of-concept of one such breakthrough was demonstrated. It was shown that nanostructured interstitial alloy-based catalysts: (a) show activity similar to Pt and Pd; (b) can be readily synthesized in desired form; and (c) show significant room temperature activity for a high volume, commercially important chemical reaction. Phase II will focus on scale-up and optimization of the nanostructured catalyst's synthesis and performance. Also, in collaboration with a leading catalyst manufacturer, bulk quantities of the catalysts will be field-tested. In order to identify and pursue spin-off commercialization opportunities, other commercially important chemical reactions that are presently catalyzed only by precious metals will be explored.

PHASE I STTR PROJECTS

Advanced Modular Power Systems Inc.
4667 Freedom Drive
Ann Arbor, MI 48108-9784

73. Improved Beta-Alumina Fabrication Using Rapid Plasma Sintering

Robert C. Svedberg
313/677-4260

Funding Profile
Date Started: July 14, 1997

FY 97 - $99,896

The Alkali-Metal Thermal to Electric Converter (AMTEC) is a high efficiency device for the direct conversion of heat to electricity. AMTEC is expected to contribute to energy savings if production costs can be lowered to levels that would stimulate demand for high volume production. The raw materials needed for AMTEC are common and inexpensive, but fabrication of the sodium beta"-alumina solid electrolyte (BASE) ceramic remains expensive. This project will demonstrate the feasibility of using microwave induced plasma heating to process the BASE, enhance the BASE quality, and dramatically reduce the high temperature processing time as well as the energy and dollar cost. In Phase I, plasma sintering techniques will be used to prepare BASE from precursor powders obtained from a variety of large scale suppliers. Parameters for fabricating standard size BASE tubes will be optimized using a statistically designed experimental matrix and the usual micro-analytical tools. Phase II will complete the fabrication process optimization and establish a rapid sintering test facility that will demonstrate the capability of the method and establish a clear path for large scale, low cost implementation.

AstroPower, Inc.
Solar Park
Newark, DE 19716-2000

74. New High-Performance GaSb-Based Thermophotovoltaic (TPV) Devices

Michael G. Mauk
302-366-0400

Funding Profile
Date Started: July 14, 1997

FY 97 - $99,995

Thermophotovoltaic (TPV) devices, used for direct conversion of heat to electrical power, currently experience high current level and functional problems such as fill factor losses and device overheating. Previous work has established the operational feasibility of InGaAsSb/GaSb homojunction TPV cells. Homojunction TPV cells are low-bandgap cells with a high spectral response, a functional requirement for TPV systems using thermal radiation. By developing a new generation of GaSb-based TPV devices, this project will improve on these devices. Phase I will optimize a double heterostructure design for significantly higher open-circuit voltages and fill-factors, and wider spectral response. Approaches for a monolithic series of interconnected TPV cells in a high-voltage array will be explored using either a proprietary epitaxial later overgrowth process, or by epitaxial film transfer techniques. Finally, an assessment of the prospects for low-cost GaSb-based TPV production will be made.

Materials and Electrochemical Research
7960 South Kolb
Tucson, AZ 85706-9237

75. High Efficiency Magnetic Refrigerators as Alternate Environmentally Safe Commercial Refrigeration Devices

Sumit K. Guha
520-574-1980

Funding Profile
Date Started: July 14, 1997

FY 97 - $100,000

The prospect of a phase-out of chlorofluorocarbons, coupled with safety and lubricity concerns with hydrofluorocarbon replacements, suggests the need for alternative refrigeration technologies. Active Magnetic Refrigeration (AMR), based on the magnetocaloric effect in which the temperature of an isolated magnetic system can change with applied magnetic field, is one such candidate. AMR has failed to reach its potential because the magnetocaloric effect, associated with the rare-earth intermetallics used as the refrigerant, is too small. A recently developed intermetallic offers the promise of a giant magnetorcaloric effect; however, its brittleness makes it unsuitable for the application. This project will concentrate on processing this brittle intermetallic into a refrigerent bed configuration using a unique powder processing approach.

APPENDIX A

ADVANCED ENERGY PROJECTS

BUDGET

	FY 1996	FY 1997	FY 1998 (REQUEST)
OPERATING	$11,652,000	$11,398,000	$7,492,000
EQUIPMENT	300,000	215,000	300,000

DISTRIBUTION OF FY 1997 FUNDS

Universities	36%
DOE Laboratories	53%
Other	11%

APPENDIX B

INVESTIGATOR INDEX

(Project Numbers)

APPENDIX C

INSTITUTIONAL INDEX
(Project Numbers)

APPENDIX D

FACSIMILE COVER SHEET

DATE: ____________

TO: Advanced Energy Projects & Technology Research Division
ER-32, GTN
U.S. Department of Energy
19901 Germantown Road
Germantown, MD 20874-1290

FROM: ____________________________
(inc. tel #)
____

SIGNATURE: ____________________________

_____ D. E. Koegel

_____ W. M. Polansky

_____ S. E. Stottlemyer

Message:

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