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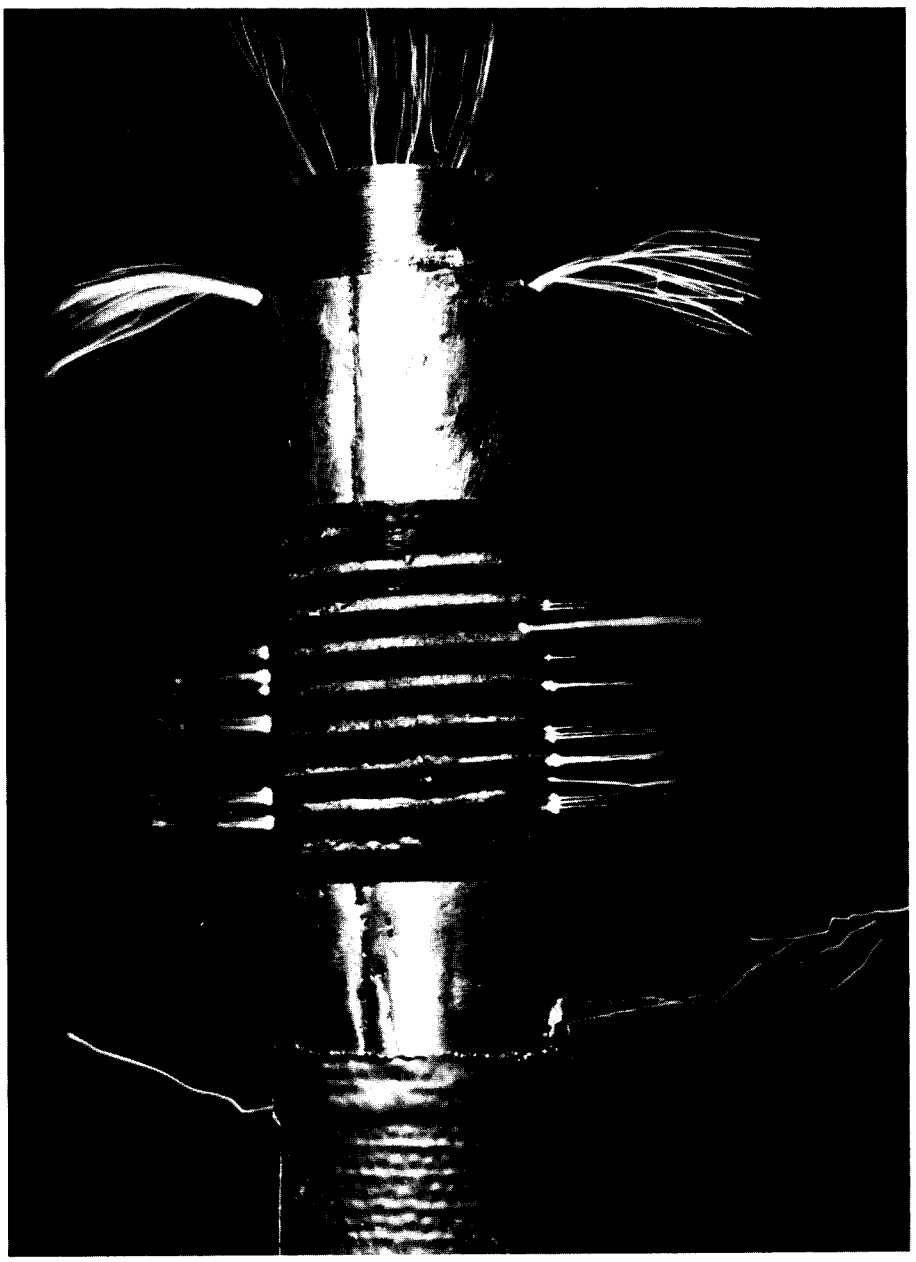
Advanced Energy Projects FY 1995 Research Summaries

September 1995



U.S. Department of Energy
Office of Energy Research
Office of Computational and
Technology Research
Advanced Energy Projects Division

Cover photograph courtesy of Leslie Bromberg, Massachusetts Institute of Technology

The photograph shows corona discharges from a magnet placed on top of a Van de Graaff generator. The helical monolithic magnet is made from bulk high temperature superconductor. The dark material is BSSCO 2212, and the light metal is silver. The silver is used for contacts. Similar magnet constructions have been used to generate persistent magnetic fields of 3T at 4.2K. (Photo by Mr. P. Thomas).

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Technology Research
Advanced Energy Projects Division
Germantown, MD 20874

TABLE OF CONTENTS

PROGRAM OVERVIEW 3

SUMMARIES OF PROJECTS 7

GRANT AND LABORATORY PROGRAMS 7

SMALL BUSINESS INNOVATION RESEARCH PROGRAM 31

APPENDICES

A. BUDGET 45

B. INVESTIGATOR INDEX 47

C. INSTITUTIONAL INDEX 49

D. FACSIMILE COVER SHEET 51

DIVISION OF ADVANCED ENERGY PROJECTS

PROGRAM OVERVIEW

CHARTER

The Advanced Energy Projects Division (AEP) provides support to explore the feasibility of novel, energy-related concepts that evolve from advances in basic research. These concepts are typically at an early stage of scientific development and, therefore, are premature for consideration by applied research or technology development programs. The AEP also supports high-risk, exploratory concepts which do not readily fit into an existing DOE program area but which could lead to applications that span scientific or technical disciplines.

The Division provides a mechanism for exploring the conversion of basic research results into applications that could impact the Nation's energy economy, or that make novel use of energy related technologies. AEP does not support evolutionary research or large scale demonstration projects. Research areas typically supported include physics, chemistry, materials, engineering, geosciences, and biotechnologies. Projects can involve interdisciplinary approaches to solve energy-related problems.

SCOPE

Projects supported by the Division arise from unsolicited ideas submitted by researchers. The portfolio of projects is dynamic, but reflects the broad role of the Department in supporting research and development for improving the Nation's energy posture. Topical areas presently receiving support are:

- Novel Materials for Energy Technology
- Renewable and Biodegradable Materials
- Exploring Uses of New Scientific Discoveries
- Alternate Pathways to Energy Efficiency
- Alternative Energy Sources
- Innovative Approaches to Waste Treatment and Reduction

Infrequently, AEP supports scientific workshops to help identify promising energy areas needing research and concept feasibility testing. This interest does not elevate the particular workshop field above the other fields covered by AEP in terms of interest for funding.

FUNDING

Projects are supported for a specified period of time, which typically does not exceed three years. In Fiscal Year 1995, the average annual funding level for an AEP project was $300,000 and the average funding period was slightly less than 36 months. Following AEP support, it is expected that each concept will be sufficiently developed and promising to attract further funding from other sources in order to realize its full potential.

SUBMISSION GUIDELINES

Unsolicited proposals can be submitted by universities, industrial organizations, non-profit research institutions, or private individuals. The Division also considers ideas or concepts submitted by researchers at national laboratories. The review process is the same for all submissions.

PREPROPOSALS

Before a formal proposal is prepared, the proposer should submit a summary (3-5 pages) of the proposed work to the Division for consideration. The summary should be sufficiently detailed to enable an informed decision

as to whether the proposed work would be programmatically suited to the charter of the Advanced Energy Projects Division. It should include descriptions of the proposed method 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." In addition to these requirements, a 200-300 word abstract describing the project should be provided.

PROPOSAL EVALUATION

Awards are based on the results of an evaluation process that includes independent reviews by external scientific and technical experts. 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?

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

- Dr. Gesina C. Carter

- Ms. Sue Ellen Stottlemyer

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This book was compiled by Sue Ellen Stottlemyer.

SUMMARIES OF PROJECTS ACTIVE IN FY 1995

GRANT AND LABORATORY PROGRAMS

There were 46 research projects in the Division of Advanced Energy Projects during Fiscal Year 1995 (October 1, 1994 - September 30, 1995). Ten projects were initiated during that fiscal year. See Appendix B for FY 1995 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, e.g., H(2)O for water and cm(2) for square centimeters.**

Alfred University
Alfred, NY 14802

1. Combustion Synthesis and Engineering of Nanoparticles for Electronic, Structural and Superconductor Applications

Gregory C. Stangle
School of Ceramic Engineering
607/871-2798

Funding Profile
Date Started: November 1, 1992
Anticipated Duration: 3 Years

FY 93 - $225,000
FY 94 - $186,000
FY 95 - $196,000

Ultrafine particles are currently difficult to produce in commercial quantities and to use in the development of dense materials with precisely controlled microstructures. The investigation will: 1) produce nanoparticles of multicomponent oxide ceramic materials by a combustion synthesis technique that is readily scaled up; 2) apply proven, in-house grain-boundary engineering methods to fine-tune microstructure evolution during densification; 3) use conventional and rapid sintering techniques to densify consolidated nanoparticle compacts; and 4) characterize the material at each stage. Expected results include: a) the synthesis of nanoparticles of complex composition for use in several applications (such as high temperature superconductivity, high surface toughness/high temperature materials, superparaelectric materials); b) the development and reduction to practice of a generic, widely applicable process; and c) the evaluation of the energy efficiency and commercialization potential of the process. The proposed study will be interdisciplinary, bringing together the areas of ceramic, electrical and chemical engineering, and will enlist three U.S.-based companies to aid in focusing the research toward the commercialization of successful research results.

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

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 susceptible 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
Ames, IA 50011

3. Design of Materials with Photonic Band Gaps

Kai-Ming Ho
Institute for Physical Research and Technology
515/294-1960

Funding Profile
Date Started: February 15, 1992
Anticipated Duration: 3 Years (Project Completed)

FY 92 - $299,000
FY 93 - $314,000
FY 94 - $297,000

This joint theoretical and experimental program is intended to design, fabricate and characterize a new class of composite materials which possess forbidden ranges of frequencies, in which electromagnetic waves cannot propagate in any direction. These materials are called "photonic crystals" and the forbidden frequencies are called "photonic gaps", and they can be regarded as photonic analogues of electronic semiconductors with electronic gaps. This class of material will exhibit many interesting physical properties, and will find important practical applications in lasers, mirrors, resonators, filters, and quantum optical devices. The theoretical effort will be directed at designing periodic dielectric structures that give the optimal frequency gap for various applications with special emphasis on the fabricability of these structures, especially in the sub-micron length scale where these materials will find applications in optical measurements. The main purpose of the experimental effort is to fabricate the structures designed by theory in the micron and sub-micron length scales, using micro-fabrication patterning and etching techniques. The structural and optical properties of these micro-structures will be characterized and studied using optical techniques. The effect of disorder, defects and structural imperfections on the propagation of electromagnetic waves through these photonic crystals will also be studied both theoretically and experimentally.

Argonne National Laboratory
9700 South Cass Avenue
Argonne, IL 60439

4. High-Flux, Large-Area Carbon-Cluster Beams for Thin-Film Deposition and Surface Modification

Dieter M. Gruen
Materials Science Division
708/252-3513

Funding Profile
Date Started: March 15, 1992
Anticipated Duration: 3 Years (Project Completed)

FY 92 - $445,000
FY 93 - $400,000
FY 94 - $355,000

The discovery of the fullerenes, and particularly of C(60), buckminsterfullerene, is an important scientific development. These kinetically stable carbon cluster molecules, allotropes of carbon, are in fact thermodynamically unstable with respect to diamond and graphite by ~5 kcal/mol C. The fact that C(60) has a vapor pressure of about 1m Torr at 500 degrees C opens up the possibility of generating high-flux, high-energy carbon-cluster ion beams for thin-film deposition (including diamond films) and surface modification. A microwave-driven electron cyclotron resonance (ECR) plasma source will be used to generate the fullerene ion beams. The ECR source combines high-ionization efficiency with low-electron temperatures (5-10eV). Typical ion current specifications for argon are 30 mA/cm(2) with a uniformity of ± 5% over a 4" diameter area. The mass transport associated with a similar current of singly ionized C(60) would correspond to 150 amps of atomic ions. The substrate impact energy will be controlled independently of the plasma parameters by biasing the substrate. End-Hall optics will be

combined with the ECR plasma to provide additional control of beam characteristics. The ECR facility will be used to synthesize and characterize, by a variety of techniques, diamond films, diamond-like films, and carbon-implanted layers on large areas with high-deposition rates. The effort is directed toward producing high-quality films at low-substrate temperatures in a manner that can be adapted to industrial processes.

Argonne National Laboratory
9700 South Cass Avenue
Argonne, IL 60439

5. Development of an Ion Replacement Electrorefining Method

Zygmunt Tomczuk
Chemical Technology Division
708/252-7294

Funding Profile
Date Started: February 15, 1992
Anticipated Duration: 3 Years (Project Completed)

FY 92 - $450,000
FY 93 - $450,000
FY 94 - $450,000

The objective of this project is to investigate promising methods for carrying out a new metal separation and purification process called ion replacement electrorefining. The challenge and program focus lie in developing a counter electrode that can serve in a sequential and, if possible, reversible manner as a cathode during metal dissolution and an anode during metal separation/deposition. The development work will be conducted with a view toward one particularly important application - the separation of spent metallic nuclear reactor fuel (or any nuclear waste material in metallic form) into its elemental constituents. The key goal is to produce a clean separation between actinide and non-actinide elements. One potential use for the ion replacement electrorefining method is the reprocessing of spent metal fuel from an Integral Fast Reactor (IFR), but it is also adaptable to the separation of transuranic elements from spent fuel and waste generated by the light water nuclear reactor (LWR) industry and the defense nuclear programs. In the case of the IFR, the proposed process represents an attractive alternative towards commercialization, in the sense that it offers a simplification of the conventional pyrometallurgical electrorefining process under development within the IFR Program. For LWR and defense waste applications, the ion replacement electrorefining method could be used in conjunction with processes that incorporate reduction of actinide element compounds (usually oxides) to a metallic form.

Argonne National Laboratory
9700 South Cass Avenue
Argonne, IL 60439

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

Gary P. Wiederrecht
Chemistry Division
708/252-6963

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 photogeneration 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 photorefractivity 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 photorefractivity and to accurately characterize the materials. Several device applications will be demonstrated.

University of Arizona
Tucson, AZ 85721

7. Creation and Destruction of C(60) and Other Fullerene Solids

Donald R. Huffman
Department of Physics
520/621-4804

Funding Profile
Date Started: March 1, 1993
Anticipated Duration: 3 Years

FY 93 - $302,000
FY 94 - $301,000
FY 95 - $302,000

This work will focus on the creation and destruction of fullerenes, for the purposes of producing new materials of interest to the Department of Energy. It is now known that, besides the famous C(60) molecule (buckminsterfullerene), hundreds of other fullerenes, with masses of up to 600 carbon atoms, are also synthesized in the Krätschmer-Huffman process. The physics underlying the creation of the fullerenes is poorly understood and the major portion of this work will be a systematic study of the process. This will involve construction of a new, fully-instrumented smoke-chamber, that will be used in a methodical exploration of fullerene yield versus production conditions. Mass-spectral analysis will be an indispensable part of this study. As part of the work, an existing time-of-flight mass-spectrometer at the University of Arizona will be upgraded for optimum performance with fullerene samples. Recent reports of the successful seeding of CVD-grown diamond films using thin films of C(70), and of the room-temperature conversion of solid C(60) into diamond powder via non-hydrostatic compression, indicate that some of the first important commercial applications of the fullerenes may involve their destruction as a means of synthesizing high-performance materials. The second major portion of this work will be a systematic study of the destruction and modification of the various fullerenes by chemical reaction, electromagnetic radiation, and electron bombardment. Transmission electron-microscopy (TEM) and electron-energy-loss spectroscopy (EELS) will be very valuable in analyzing the results of these destructive tests, and a portion of the proposed funding will support this work at a TEM / EELS facility located at the University of Arizona.

Auburn University
Auburn University, AL 36849

8. 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 work is aimed at conducting the basic and exploratory research which will allow the development of high intensity, discrete frequency infrared sources which 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 also 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.

Brooklyn College of City University of New York
Brooklyn, NY 11210

9. Solar Detoxification of Aquatic Systems With Porous Photocatalysts

Micha Tomkiewicz
Physics Department
718/951-5357

Funding Profile
Date Started: November 15, 1991
Anticipated Duration: 3 years (Project Completed)

FY 92 - $118,000
FY 93 - $127,000
FY 94 - $131,000

The objective of this project is two fold: (a) To investigate the feasibility of using a porous structure of a side bandgap semiconductor as a portable photocatalyst for photodegradation of organic pollutants in an aqueous environment; and (b) establish the correlation between the morphology of the porous photocatalyst and its efficiency in the photocatalytic process. Initially, efforts will be concentrated on the photocatalytic decomposition of two classes of organic materials: (a) Hydrocarbons, both light aliphatic and light aromatics, such as benzene and toluene. This work will be aimed primarily at water decontamination due to oil spills. (b) Salicylates. These are soluble ionic compounds that are being proposed in some quarters to serve as standards for the efficiency of various water purification schemes. The initial choices for the photocatalyst are porous TiO(2) films or beads that will be prepared either by the sol-gel method or by thermal decomposition of organic titanates, to make them low density enough to float in an aqueous environment. The principal tools in analyzing the porosity and the pore structure will be image processing in conjunction with optical and electron microscopies, small-angle x-ray scattering and impedance measurements. The reactants and the reaction products will be analyzed by absorption spectroscopy, by gas and liquid chromatography, and by electrodes specific to oxygen and carbon dioxide. Slow kinetic studies will be conducted by monitoring the time evolution of disappearance of the reactants and appearance of the products. Kinetic studies on a faster time scale will be conducted by flash-photolysis absorption measurements and time resolved luminescence. Parallel to the experimental work, computer simulations of the photocatalytic process on random porous photocatalysts and on porous deterministic fractals will be conducted.

University of California, Los Angeles
405 Hilgard Avenue
Los Angeles, CA 90024

10. Experimental, Theoretical and Computational Study of Frequency Upshift of Electromagnetic Radiation Using Plasma Techniques

Chan J. Joshi
Electrical Engineering Department
310/825-7279

Funding Profile
Date Started: January 15, 1991
Anticipated Duration: 4 Years (Project Completed)*

FY 91 - $250,000
FY 92 - $250,000
FY 93 - $250,000

In this project, a new class of coherent electromagnetic radiation generation devices that, in principle, can cover the range of frequencies from microwaves to the vacuum ultra-violet, will be investigated both theoretically and experimentally. In this method the frequency of the incident electromagnetic wave is upshifted by suddenly lowering the refractive index of the medium through which the wave is propagating. This can be done by rapidly ionizing the medium and forming a plasma. Various regimes will be investigated:

(a) Spatially uniform ionization (or flash ionization). If the source wave is propagating through a medium that is uniformly ionized in time, then the wavenumber of this source wave is fixed, but the frequency can increase. This technique is particularly useful for generating tunable electromagnetic radiation in the mm wave range. *(b) Frequency upshift by a moving ionization front.* By sending an ionization front, it is also possible to upshift the source wave frequency. If the plasma frequency is greater than the source frequency, this technique can generate frequency upshifts that are much greater than the flash ionization technique. This technique is suited to generate far-infrared and infrared radiation. An applications study will also be undertaken to identify technologies which would likely be impacted by these sources.

*Includes 12 month no-cost extension

University of California, Los Angeles
405 Hilgard Avenue
Los Angeles, CA 90024

11. Synchronous Picosecond Sonoluminescence: Developing and Characterizing a New Light Source

Seth J. Putterman
Department of Physics
310/825-2269

Funding Profile
Date Started: December 15, 1991
Anticipated Duration: 3.5 Years (Project Completed)*

FY 92 - $388,000
FY 93 - $275,000
FY 94 - $194,000

It has recently been discovered at the UCLA acoustics laboratory that the passage of a sound wave through a liquid leads to the ultra-precise clock-like emission of flashes of light. The power of the individual flashes is greater than 1 milliwatt and their width is less than 100 picoseconds. This effect is due to a spontaneous yet controllable concentration of sound energy by a factor of one trillion. The goal of this project is to perform those measurements which will elucidate the mechanism responsible for this off-equilibrium phenomenon (that has been named synchronous picosecond sonoluminescence). Toward this goal, the time and spatial resolution of the flashes will be measured along with the time development of the spectrum. Correlations and possible coherence will be searched for in the radiated light. Efforts will be made to measure the spectrum of microwave, radio frequency and far ultra-violet radiation. The degree of synchronicity will also be probed. These efforts will lead to the development of a variable width, variable intensity picosecond light pulser. By understanding the novel cooperative effects that cause synchronous picosecond sonoluminescence, insight will be gained as regards the means whereby large controllable energy concentrations could be achieved in other systems.

*Includes 6 month no cost extension

University of California, Santa Barbara
Santa Barbara, CA 93103

12. Photo-Induced Electron Transfer From a Conducting Polymer to Buckminsterfullerene: A Molecular Approach to High Efficiency Photovoltaic Cells

Paul Smith
Materials Department
805/893-8104

Funding Profile
Date Started: August 15, 1993
Anticipated Duration: 3 Years

FY 93 - $171,000
FY 94 - $283,000
FY 95 - $446,000

The recently-discovered photoinduced electron transfer, with subpicosecond transfer rate, in composites of a conducting polymer, MEH-PPV, and a molecular acceptor, buckminsterfullerene, C(60), opens a new direction and a new opportunity for photovoltaic research. Since the charge transfer takes place ~1000 times faster than the radiative and/or non-radiative decay of photoexicitations, the quantum efficiency for charge transfer and charge separation is near unity. Photoinduced electron transfer across the donor-acceptor rectifying heterojunction offers potential for solar cell applications, using materials that exhibit a unique combination of properties: electronic and optical properties of semiconductors and metals in combination with the attractive mechanical properties and the processing advantages of polymers. The potential advantages of an all-polymer heterojunction solar cell include the following: low cost (literally fabricated from solution); large area; and flexible (components are

polymers that can be solution cast onto polymer substrates). The goal of the proposed research is to build upon this novel molecular approach to photoinduced charge separation and charge transfer, with quantum efficiency approaching unity, and to create a research and development program that will enable the production of efficient, flexible, "plastic" solar cells that can be implemented in large areas.

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

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

The objective of this research program 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

Henryk Temkin
Department of Electrical Engineering
303/491-6018

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 photogenerated 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 can be 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.

General Electric Company
Schenectady, NY 12301-0008

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

David W. Skelly
Corporate R&D Center
518/387-6534

Funding Profile
Date Started: January 15, 1994
Anticipated Duration: 3 Years

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 program 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.

Johns Hopkins University
Baltimore, MD 21218

16. 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: 3 Years

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 the 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.

Lawrence Berkeley Laboratory
Berkeley, CA 94720

17. Compact MeV Ion Implanter

Simone Anders
Plasma Applications Group
510/486-6745

Funding Profile
Date Started: February 15, 1994
Anticipated Duration: 3 Years

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 Laboratory
Berkeley, CA 94720

18. 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

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 properties with

addition of Mg. The nitrogen concentration of the films was greatly increased, by using a reactive ion-beam process, thus eliminating the primary background defect concentration. Upon attaining threshold levels of conductivity and mobility, it was discovered that good quality material 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 Livermore National Laboratory
Livermore, CA 94550

19. Pulsed Plasma Processing of Effluent Gases

J. N. Bardsley
510/422-6008

Funding Profile
Date Started: July 10, 1992
Anticipated Duration: 3 Years (Project Completed)

FY 92 - $222,000
FY 93 - $108,000
FY 94 - $330,000
FY 95 - $330,000

A study will be carried out of the science underlying the use of pulsed electrical discharges for the simultaneous removal of NO(x), SO(2) and soot from diesel engine exhausts. The goals involve major advances in the understanding of breakdown mechanisms in coronal discharges, the elucidation of the chemical reaction schemes responsible for the conversion of the pollutants to benign molecules, experimentation with novel devices, preliminary analysis of the scaling laws, and economic and environmental considerations relevant to the transfer of this technology from the laboratory. The research will be performed by a multidisciplinary team from the Physics, Electrical Engineering, and the Chemistry and Materials Science Departments.

Lawrence Livermore National Laboratory
Livermore, CA 94550

20. Solid State Multi-Layered Batteries

Richard M. Bionta
510/423-4846

Funding Profile
Date Started: October 15, 1993
Anticipated Duration: 2 Years

FY 94 - $419,000
FY 95 - $296,000

The purpose of this project is to develop and study thin film solid-electrolyte batteries fabricated by the advanced multilayer sputtering techniques developed for x-ray optics. This technique allows the battery to be constructed in situ by depositing the anode, electrolyte, and cathode as distinct layers with several computer controlled magnetron sputtering sources. Solid-electrolyte batteries have long been attractive because of their shelf-life and compatibility with severe environments. The discovery of new materials for cell construction has resulted in increased solid state battery research. Recently, rechargeable lithium cells that operate at ambient temperature have been developed based on ionically conducting solid polymer electrolytes. This project will concentrate on the development of thin-film solid-electrolyte cells constructed of lithium based inorganic materials fabricated by multilayer sputtering. The ability of this fabrication technique to discretely layer or compositionally grade thin films provides a unique opportunity to investigate the effect of electrode-electrolyte interface structure on cell performance. Finally, the computer control associated with this fabrication technique will allow the deposition of multiple cells in a bipolar configuration with either series or parallel connection. It is anticipated that this research will directly lead to practical applications of thin film solid state batteries as integrated power sources for modern electronic circuits (i.e. microsensors, memory elements, displays, and timers).

Lawrence Livermore National Laboratory
Livermore, CA 94550

21. Thermoelectric Quantum Wells

Joseph C. Farmer
510/423-6574

Funding Profile
Date Started: January 15, 1994
Anticipated Duration: 3 Years

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. Multilayers 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)Geo(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

22. Porous Carbons: Controlling Structure, Composition and Performance

Richard W. Pekala
Chemistry and Materials Science Department
510/422-0152

Funding Profile
Date Started: March 15, 1994
Anticipated Duration: 3 Years

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 ultrafine 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 cycleability 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 multifunctional 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.

Los Alamos National Laboratory
Los Alamos, NM 87545

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

Reed J. Jensen
505/667-9909

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

24. Synthesis and Properties of High Strength Nanolayered Composites

Michael Nastasi
505/667-7007

Funding Profile
Date Started: February 15, 1993
Anticipated Duration: 3 Years

FY 93 - $150,000
FY 94 - $315,000
FY 95 - $330,000

The objective of this project is to synthesize and evaluate ultra high strength vapor-deposited nanoscale materials both in the monolithic and composite form. Such materials have been shown to posses strengths that are within a factor of three or four of the theoretical shear strength modulus. Synthesis of nanoscale materials presents the opportunity to develop a basic understanding of the deformation and fracture mechanisms that operate close to the theoretical limit of strength of materials to enable a new technological breakthrough, namely mechanical miniaturization. The availability of the fine-scale ultra high strength materials would provide the basis for fabricating, among others, miniature activators, springs, and diaphragms, for biomedical or sensor applications. The primary performance task will be to synthesize ductile materials with ultra high strength for application in mechanical miniaturization.

Los Alamos National Laboratory
Los Alamos, NM 87545

25. Experimental and Theoretical Studies of Inertial-Electrostatic Confinement

Richard A. Nebel
505/667-7721

Funding Profile
Date Started: November 1, 1991
Anticipated Duration: 3 Years (Project Completed)

FY 92 - $400,000
FY 93 - $400,000
FY 94 - $392,000

A comprehensive study of inertial-electrostatic confinement (IEC) will be conducted. IEC is a plasma confinement scheme for fusion applications based on electrostatic fields. Unlike conventional magnetic confinement fusion, IEC devices produce fusion via non-Maxwellian beam-beam interactions; the kinetic energy of the beam ions being approximately the same as the potential on the grid. Experimental work complemented and guided by theoretical analysis will be pursued. The experimental effort will be centered at the University of Illinois. Experimental diagnostics will glean data to determine the spatial dependence of both the neutron-emission source and the associated electrostatic potential. These data will

be used to assess and improve the understanding of IEC and to test new physics concepts that may enhance ion compression and collision rates in such devices. The computational strengths of Los Alamos National Laboratory (LANL) together with the phenomenological modeling capabilities of Energy/Matter Conversion Corp., (EMC2) will be used to achieve this mission. A three-dimensional semi-implicit Particle-In-Cell (PIC) code is currently being developed at LANL that is appropriate for modeling both the IEC experiments and conventional as well as newly developed phenomenological physics models of interest in their interpretation. Possible instabilities will be studied in order to determine their effect upon the electrostatic confinement. The primary goals will be to determine conditions for maximum ion confinement and to define appropriate experimental regimes for their test.

Massachusetts Institute of Technology
Cambridge, MA 02139

26. Superconducting Bitter Magnets

Leslie Bromberg
Plasma Fusion Center
617/253-6919

Funding Profile
Date Started: May 1, 1993
Anticipated Duration: 3 Years

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 on 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.

University of Michigan
Ann Arbor, MI 48109

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

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

Funding Profile
Date Started: November 1, 1992
Anticipated Duration: 3 Years

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 microstructural 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 microstructure that is comparable to that produced by neutron irradiation in a fraction of the time and at a fraction of the cost. This program is designed to uncover the effects of grain boundary impurity segregation, chromium depletion, and the irradiated microstructure on ASK. 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 microstructure 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.

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

28. PV-Powered, Electrochromic Windows

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

Funding Profile
Date Started: February 15, 1994
Anticipated Duration: 3 Years

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 daylighting control functions which will reduce heating, cooling, and lighting energy usage in the building. The self-powered 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

29. Hot Carrier Solar Cells

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

Funding Profile
Date Started: February 15, 1994
Anticipated Duration: 3 Years

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 photocurrent and photovoltage of the cell can be separately controlled and optimized, unlike the conventional p-n photovoltaic cell where the photocurrent 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.

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

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

Lawrence L. Kazmerski
Photovoltaics and Basic Sciences Division
303/384-6600

Funding Profile
Date Started: July 10, 1994
Anticipated Duration: 3 Years

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

This project uses scanning probe microscopies 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 program 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. The program provides the first atomic engineering directed toward these III-V materials. It further provides fundamental information of the nature of defects, their electrooptical 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 electrooptical 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.

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

31. Photochemical Solar Cells

Arthur J. Nozik
303/384-6603

Funding Profile
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 photostability. 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.

University of Nebraska
Lincoln, NE 68588-0111

32. *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: 3 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 program 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 spacially-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. Multilayers 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 program 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.

Oak Ridge National Laboratory
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Oak Ridge, TN 37831

33. Novel Composite Coatings for High Temperature Friction and Wear Control

Theodore M. Besmann
Metals and Ceramics Division
615/574-6852

Funding Profile
Date Started: November 1, 1991
Anticipated Duration: 3 Years (Project Completed)

FY 92 - $428,000
FY 93 - $250,000
FY 94 - $260,000

The development of improved, self-lubricating materials is critical for enabling progress in many industrial sectors: transportation, industrial machinery, business machines, aerospace, and defense. Its impact on the economy will therefore

be large and diverse, spanning devices from high-temperature turbine engines to moving parts in heat-treatment systems for integrated circuitry. Chemical vapor deposition (CVD) techniques offer the opportunity to create very uniform self-lubricating composites which slowly wear away to expose pockets of lubricants which then spread across the surface. In CVD, gaseous reactants are allowed to flow over a heated substrate where they react and deposit a solid coating. Solid lubricants have higher use temperatures and higher load-bearing capacities than do liquid lubricants. Consequently, they find use in applications where liquid lubricants prove inadequate. It has been noted that because buckminsterfullerene [C(60)] is a spherical macromolecule and is thought to be very stable and slow to react with other substances, it should make an excellent lubricant. This project utilizes the controlled wear of a hard matrix to reveal the embedded high-temperature, solid lubricant. Such a composite coating would be produced by CVD, which has been demonstrated capable of producing multiphase coatings of controlled composition and microstructure. The C(60) phase cannot be simultaneously formed during deposition, as can other of the proposed lubricants. The material can be incorporated into a coating, however, by entrainment in the coating gases.

Princeton University
Princeton, NJ 08544-1009

34. Optimally Controlled Interior Manipulation of Solids

Herschel Rabitz
Department of Chemistry
609/258-3917

Funding Profile
Date Started: November 19, 1992
Anticipated Duration: 3 Years

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.

Purdue University
1295 Potter Engineering Center
West Lafayette, IN 47907

35. Zeolite Catalysis in Conversion of Cellulosics

George T. Tsao
Laboratory of Renewable Resources Engineering
317/494-7024

Funding Profile
Date Started: February 15, 1992
Anticipated Duration: 3 Years (Project Completed)

FY 92 - $255,000
FY 93 - $235,000
FY 94 - $244,000

The use of zeolite catalysts may improve conversion of cellulosics in two important ways, namely (a) reduction of glucose inhibition of cellulase activities; and (b) efficient conversion of xylose into xylulose and then ethanol. This project will study adsorption of carbohydrates, hydrolysis of oligosaccharides, and aldose-ketose isomerization catalyzed by zeolites under various conditions. High pressure liquid chromatography, nuclear magnetic resonance and infrared measurements will be used to detect sugars and to examine their interactions with the zeolites. These studies will help to elucidate the mechanism, kinetics, diffusion, and equilibrium of the reactions as they are affected by the presence of zeolites. Zeolite-promoted reactions including isomerization and oligomer hydrolysis can be coupled with biological reactions including enzymatic hydrolysis and yeast fermentation for the above-mentioned improved overall conversion of cellulosics.

Sandia National Laboratories
Albuquerque, NM 87185-0346

36. 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 into 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 proposal is to develop such multi-alloy structures grown by meal 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 wells 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 modelling, 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 electroluminescence spectra, current-voltage, and light-current characteristics.

Sandia National Laboratories
Albuquerque, NM 87185-0346

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

Regan W. Stinnett
505/845-7488

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 based on surface melting followed by rapid thermal quenching by thermal diffusion into the underlying, untreated bulk material. This process produces non-equilibrium microstructures, 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.

Science Research Laboratory
1150 Ballena Boulevard, Suite 100
Alameda, CA 94501

38. The Plasma Centrifuge (A Compact, Low Cost, Stable Isotope Separator)

Philip Greene
617/547-1122

Funding Profile
Date Started: September 15, 1991
Anticipated Duration: 42 Months (Project Completed)

FY 91 - $495,000
FY 92 - $441,000
FY 93 - $317,000

The objective of this project is to make practical a new type of isotope separator called the Plasma Centrifuge. The Plasma Centrifuge is based on the concept of a cylinder of ionized matter (plasma) contained by a magnetic field and set into rotation by application of an electromagnetic body force. The typical embodiment consists of a rotating column that is fed by a vacuum arc plasma source at one end. As the plasma streams towards the other end of the chamber, centrifugal forces cause the heavier isotopes of the plasma ions to move nearer the periphery of the rotating column, resulting in partial separation between the constituent isotopes. Collectors placed at the other end of the column can collect either the outer portion that is enriched in the heavier isotope; or the inner portion that is enriched in the lighter isotope, as desired. This Plasma Centrifuge apparatus fits into a small room and can enrich dozens of isotopes with a throughput of about 1-3 grams/hour of enriched product. Such a capability would make this centrifuge a useful new separator to supply the U.S. demand for a variety of enriched isotopes that are badly needed in these quantities in the fields of basic research in physics/chemistry/geology/ medicine and in medical diagnostics radiological practice. The cost, modularity and size of this approach makes the Plasma Centrifuge a potential replacement for CALUTRONS, which are today's primary source of supply of enriched isotopes.

Stanford University
Stanford, CA 94305

39. Nonlinear Optics in Doped Fibers

Richard H. Pantell
Electrical Engineering Department
415/723-2564

Funding Profile
Date Started: May 1, 1992
Anticipated Duration: 3 years (Project Completed)

FY 92 - $364,000
FY 93 - $363,000
FY 94 - $366,000

The objective of this project is to develop a novel and simple technology for optical, all-fiber switches based on the third order nonlinear effect in doped, single-mode fibers. The principle behind these devices is that, when exciting a transition near resonance, the electronic distribution changes and so does the contribution of this transition to the refractive index of the material. This effect exists in pure silica, but it is extremely weak, and in undoped, pure silica fibers. Tens of watts and tens of meters of fiber are required to induce the phase shift of pi needed for switching. The novelty of this

approach is to use a fiber doped with an appropriate impurity and excite it optically near an absorption resonance of this impurity to produce strongly enhanced nonlinear susceptibilities. Modeling shows that it is then possible to reduce the pump and length requirements by several orders of magnitude each, and to produce a pi phase shift in centimeter lengths with milliwatts of pump power. The ultimate thrust of this project is to investigate this effect with a variety of impurities exhibiting high oscillator strength transitions to produce both high speed and very short devices. For picosecond response times, the reduction in the pump power-fiber length product is predicted to be 7 - 8 orders of magnitude over undoped silica. Slower but useful devices will also be investigated using well-understood erbium and neodymium-doped fibers that have been extensively studied as lasers and amplifiers but not as nonlinear switches. This investigation is anticipated to open the door to the first low-power, ultra-short switches and modulators made with single-mode optical fibers, operated with a low-power, long-lifetime laser diode. Such components are not currently available in a form compatible with fiber optic systems, either from fiber-based or integrated-optic based elements. There are a variety of energy applications for the proposed research, including oil exploration, control of power substations, and management of consumer distribution systems. Interactions with several companies are planned throughout this study for directivity, technology transfer, and manufacturing of some of the devices tested under the program.

TecOne
1803 Sageway Drive
Tallahassee, FL 32303

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

Louis R. Testardi
904/562-9789

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

FY 95 - $170,000
FY 96 - $166,000
FY 97 - $170,000

'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 program 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

41. 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: 3 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 ultralow 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.

University of Texas
Odessa, TX 79762-8301

42. 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: 3 Years

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 multistep 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 multistep reaction design, a single pure product such as hexane may result instead of a crude fuel mixture which results from pyrolysis methods.

University of Washington
Seattle, WA 98195

43. 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: 2 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 concepts. 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. A two year research program designed to explore the advantages of a liquid nitrogen energy storage system for automotive propulsion will be carried out. 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.

University of Washington
Seattle, WA 98195

44. 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: 3 Years

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 gasdynamic 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. The research program 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.

Washington State University
Pullman, WA 99164-2814

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

Henry C. Kapteyn
Department of Physics
509/335-4671

Funding Profile
Date Started: April 19, 1993
Anticipated Duration: 3 Years

FY 93 - $156,000
FY 94 - $158,000
FY 95 - $131,000

The goal of this project is to implement a new approach for producing ultrashort 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 multiphoton 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.

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

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

Michael R. Seal
Department of Technology Engineering
334/650-3045

Funding Profile
Date Started: August 1, 1994

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

In an internal combustion engine, fuel is mixed with air and periodically exploded. Because the explosions are of very short duration, the fuel 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 benchtop 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.

SMALL BUSINESS INNOVATION RESEARCH PROGRAM

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 1995 was about $69 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 1995 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 1995, the Advanced Energy Projects Division (AEP) managed fourteen Phase I SBIR projects, awarded under the topic, "Novel Materials for Sustainable Energy Development," in the 1995 SBIR Program Solicitation. AEP is also managing five Phase II SBIR projects selected from grant applications submitted to the topic, "Design and Applications of Novel Materials", in the 1993 DOE SBIR Program Solicitation, and six Phase II SBIR projects selected from the 1994 DOE SBIR Program Solicitation, of which three selected were selected under the topic, "Green Car: Scientific Approaches to Automotive Applications (subtopic - Novel Approaches to Propelling Automobiles)" and three selected under the topic, "Design and Applications of Novel Materials".

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

47. Low Cost, Contamination-Tolerant Electrocatalysts for Low Temperature Fuel Cells

Jaeseok Ryu
508/481-5058

Funding Profile
Date Started: September 1, 1995

FY 1995 - $74,998

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 roadblocks for large scale consumer applications of fuel cell technology is the high cost and limited supply of the noble metal-based catalysts, and catalyst poisoning. Metal carbides, such as molybdenum carbide and tungsten carbide (or their mixtures) exhibited high catalytic activity toward electro-oxidation of the methanol. In addition, these catalysts are tolerant of carbon monoxide contamination in the reaction zone. A major drawback associated with these materials is the difficulty in producing materials with high surface area. Usually, a very costly high temperature reduction and carburization, or a high energy process, such as ion implantation, is used to prepare high-surface-metal carbides. In Phase I, nanoscale group VI metal carbides will be produced utilizing nonconventional surfactants in a chemical reducing process. A technique for controlling composition, morphology, and particle size of these materials will be developed. The produced metal carbides will be evaluated with respect to surface area, particle size, particle morphology, size distribution, composition and crystallinity, presence of impurity phases, and localized electronic energy levels in the surface. Furthermore, the electrocatalytic activity of the nanoscale metal carbide produced will be investigated for the hydrogen and methanol oxidation.

Cordec Corporation
P.O. Box 188
Lorton, VA 22199-0188

48. Laser Consolidation of SiC/Ti Metal Composite Turbine Rings

Raymond J. Weimer
703/550-8044

Funding Profile
Date Started: September 1, 1995

FY 95 - $75,000

The extraordinary potential of high temperature composite materials to meet the engineering design challenges presented by advanced turbine engines is well known. Implementation has been seriously impeded by high cost and fabrication difficulties. Recently, continuous microcomposite monofilaments were produced by physical vapor deposition (PVD) methods to provide an improved alternative to drum-wound foil/fiber or plasma-sprayed monotapes. Such metal matrix composite (MMC) precursors are highly uniform and reproducible. Moreover, the local fiber volume fraction is precisely that desired in the consolidated macrocomposite structure, making the precursor ideal for a precision fiber placement and consolidation scheme. In the planned work, a unit consolidation process will be modeled and developed using laser energy to effect consolidation of continuous silicon carbide/titanium PVD MMC precursor wires. The feasibility of the approach will be demonstrated in Phase I by fabricating a subscale compressor ring for turbine engine applications. Phase II will explore the dimensions of the processing window, relying on parametric studies to model the consolidation response surface and produce a high-quality, full-scale demonstration ring.

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

49. Integrated Catalyst/Collector Structure for Regenerative PEM Fuel Cell

Larry L. Swette
617/899-7270

Funding Profile
Date Started: September 1, 1995

FY 95 - $75,000

Dedicated proton-exchange membrane (PEM) fuel cells, electrolyzers and single-unit regenerative fuel cells (RFCs) have been identified by the Department of Defense as simplified technology of potential benefit to the electric vehicle and energy storage programs. The innovation planned for investigation in Phase I is the development of a novel gas-diffusion electrode/current-collection interface (GCI) structure to yield superior performance, stability, and simplicity at the positive electrode of these PEM electrochemical cells. The structure is based on development of a stabilized, unique metal sinter that provides PEM fuel cell catalytic activity and facilitates bulk fluid distribution. It will be evaluated in Phase I and implemented in Phase II. The anticipated results are improved bifunctional performance at the positive electrode and similar construction both of the GCI and the bipolar plate, leading to reduced complexity of the system and greater feasibility for a single-unit PEMRFC.

Harvest Technology
14431 Ventura Boulevard, #273
Sherman Oaks, CA 91423

50. Molten Film High-Intensity Paper Drying

David Warren
818/386-1355

Funding Profile
Date Started: September 1, 1995

FY 95 - $74,993

A novel, energy-efficient, high-intensity drying process will be developed to enhance overall productivity in the paper making operation. The drying process involves direct contact between a wet paper web and a molten metal heat transfer fluid to achieve an order of magnitude increase in the drying rate compared to conventional evaporative dryers. The molten film high-intensity dryer replaces the complex multi-cylinder apparatus and air handling systems of conventional paper dryers with a single, integrated, heat exchange device resulting in a significant reduction in dryer size and cost. Because the high-intensity drying process does not depend on the heating of large quantities of ventilation air to remove moisture from the paper machine room, a 10 to 30% increase in thermal economy is attained. Prior attempts to achieve high-intensity drying using heated belts, platens, or press rolls to transfer drying heat to the paper web have been constrained by limitations in production speed, operating flexibility, and product quality. The use of molten metal alloys as the thermal drying medium overcomes these limitations by providing a simplified dynamic method of high-intensity heat input having relevance to a broad spectrum of drying applications. Phase I will demonstrate the feasibility of the molten film drying cycle, and experimental tests will be conducted to measure heat fluxes and dried paper mechanical properties obtained using a dynamic molten film dryer test rig. Phase II will involve engineering development of the high-intensity molten film dryer to address critical issues for commercial scale-up.

ISM Technologies, Inc.
9965 Carroll Canyon Road
San Diego, CA 92131

51. Conformal Source Ion Implantation

James R. Treglio
619/530-2332

Funding Profile
Date Started: September 1, 1995

FY 95 - $74,796

Plasma source ion implantation (PSII) has drawn a great deal of interest as a means of surface modification of large molds and dies. While having proven successful in extending the wear life of such tools and other components, the process has two fundamental drawbacks: no secondary electron suppression, and a high level of dependence on the formation and growth of a plasma sheath. The lack of secondary electron emission leads to extremely high, and very dangerous, levels of X-ray emission and very low system energy efficiency. Inability to control the plasma sheath leads to poor

process control. Therefore, the commercial value of the process is greatly limited. This project will develop a variation of PSII, Conformal Source Ion Implantation, or CSII, that will have (1) secondary electron suppression and (2) control of the formation and growth of the plasma sheath. In Phase I, experiments will be conducted on the ability of the CSII concept to suppress emission of secondary electrons. Demonstration of control of formation and growth of the plasma sheath will be left for Phase II.

Lynntech, Inc.
7610 Eastmark Drive
Suite 105
College Station, TX 77840-4024

52. Synthesis and Application of Novel Electrode Materials for Use in Protron Exchange Membrane Fuel Cells Capable of Using Simple Organic Fuels and Fuel Reformate

King Tsai Jeng
409/693-0017

Funding Profile
Date Started: September 1, 1995

FY 95 - $75,000

The goal of this Phase I project is to demonstrate the feasibility of using novel electrode materials in proton exchange membrane (PEM)-based fuel cells as versatile power sources. Fuel cells bring about direct conversion of stored chemical energy to electrical energy with efficiencies much higher than those of Carnot engines and with little or no production of pollutants. The PEM-based fuel cell system is one of the leading candidate fuel cell power sources for many commercial and military applications. Although small organic compounds, such as methanol, formaldehyde, and formic acid as well as fuel reformate have great potential for use as the main fuels in PEM-based fuel cells in the near future, the problem of electrocatalyst poisoning caused by the organic intermediates, such as strongly adsorbed carbon monoxide formed during the electrochemical oxidation process, makes the use of these compounds still impractical. New electrocatalysts, advanced electrode materials and fabrication, and other enhancement approaches are needed to obtain satisfactory operation. The objective of this project is to synthesize novel electrode materials and to develop methods for the fabrication of poison-resistant electrodes. The use of such electrode materials in PEM-based organic-air fuel cells will be evaluated to determine their potential in solving electrode poisoning problems. Success in this effort will make the use of simple organic fuels and hydrogen derived from steam reformed methanol in PEM fuel cells possible and will result in the production of long service life, high energy density, low cost, and more competitive fuel cell power sources.

Media and Process Technology, Inc.
1155 William Pitt Way
Pittsburgh, PA 15238

53. Steam Resistant Hydrogen Selective Ceramic Membranes for Fuel Cell Applications

Paul K. T. Liu
412/826-3711

Funding Profile
Date Started: September 1, 1995

FY 95 - $74,684

From an environmental perspective, it is recognized that fuel cells are theoretically more efficient and produce lower emissions of sulfur oxides and nitrogen oxides than conventional combustion technology for power generation. Although fuel cell technology is commercially available (e.g. phosphoric acid), a number of technical hurdles must be overcome to improve their performance, not the least of which is the economical generation of fuel. A potential source of hydrogen that has been widely investigated is the methane steam reforming process. The production economics can be much improved with the application of advanced membrane reactor technology. Hydrogen selective ceramic membranes would be ideally suited to this application. At the expected reaction temperatures of 450 to 650 degrees C, these membranes display: (1) H(2)/CH(4) separation factors of 100 to 400; (2) superior H(2) permeance (ca. 5 to 10 m(3)/m(2)/hr/bar); and (3) excellent resistance to common natural gas steam impurities (e.g.: sulfur dioxide, hydrogen sulfide). Unfortunately, the hydrogen permeance of these membranes is reduced significantly as a result of sintering by steam at the reaction temperature. Steam-resistant ceramic membrane technology will be explored in Phase I of this project. In addition the potential economic impact will be quantified through mathematical modeling and simulation

based upon the experimentally determined hydrogen permselectivity.

Millennium Materials, Inc.
120 Sherlake Drive
Knoxville, TN 37922-2307

54. Silicon Hexaboride Reinforced Aluminum Ingot Material Development for the Transportation Industry

Samuel C. Weaver
615/691-2170

Funding Profile
Date Started: September 1, 1995

FY 95 - $75,000

The high specific strength of metal matrix composites (MMCs) has the potential for reducing vehicle mass, thereby reducing domestic oil consumption. MMCs are of interest for use in brake rotors, calipers, steering knuckles, connecting rods, and other automotive components. Silicon carbide reinforced aluminum (SiC/Al) can be cast, but silicon carbide (3.2 g/cc), which is more dense than molten aluminum (2.4 g/cc), settles to the bottom of the melting crucible. The composite melt requires constant stirring, introducing hydrogen, oxide inclusions, and air bubbles. This Phase I project will develop and produce silicon hexaboride reinforced aluminum, SiB(6)/Al, for automotive and other transportation industry applications. The density of silicon hexaboride (2.43 g/cc) is much closer to that of molten aluminum and should have significantly less tendency to settle during the casting operations. Ingots of SiB(6)/Al will be manufactured and melted to study the stability of particulate distribution. Test specimens of this new material will be cast and analyzed for physical and mechanical properties. Phase I will be used to define a comprehensive Phase II project that will refine the manufacturing process and produce automotive components for evaluation.

Nanomaterials Research Corporation
10960 North Stallard Place
Tucson, AZ 87537

55. Nanostructured Interstitial Alloys as Catalysts for Direct Energy Applications

Tapesh Yadav
602/575-1354

Funding Profile
Date Started: September 1, 1995

FY 95 - $75,000

Interstitial alloys have excellent mechanical properties, thermal properties, and resistance to corrosion. These characteristics and the ready availability of the alloys make them useful in a variety of structural components and cutting tools. These alloys also have unique electronic and magnetic properties that, when combined with their natural mechanical and chemical properties, can lead to commercially useful catalysts with direct energy applications. A particularly significant application of great commercial significance is their potential as replacement catalytic materials for widely-used precious metals such as platinum, iridium, rhodium, and palladium. Not only are precious metals expensive (price ranging from $3,000 to $15,000 per pound), but the United States imports large amounts of these metals to meet the demand for energy and environmental catalysts. Thus, catalysts based on interstitial alloys that can replace precious metals are a significant opportunity. During Phase I, the proof-of-concept that nanostructured interstitial alloys with desirable characteristics can be synthesized will be demonstrated. The catalytic characteristics of the nanostructured interstitial alloys for commercially important reactions will also be evaluated. Phase II will develop, optimize, and field test nanostructured catalysts. Phase III will commercialize the technology.

Precision Combustion, Inc.
35 Science Park
New Haven, CT 06511

56. Integrated Catalyst/Substrate for Catalytic Combustion

William Pfefferle
203/786-5215

Funding Profile
Date Started: September 1, 1995

FY 95 - $75,000

Catalytic combustion offers significant advantages for high efficiency, ultra-low emissions combustion applications in gas turbine engines, burners, incinerators, and even internal combustion reciprocating engines. With catalytic combustion, nitrogen oxide emissions can be effectively eliminated without aftertreatment, by enabling combustion at a temperature below the NO(x) formation level. Combustion efficiency is maintained at a high level and carbon monoxide/unburned hydrocarbon emissions are kept low. To date, limits on the ability of the catalyst surface and its substrate to survive high temperatures (e.g., 1000 to 1600 degrees C) in reactive atmospheres have severely restricted practical applications. Body doped, high temperature oxide ceramics such as hexaaluminates offer the promise of a thermally stable, catalytically active monolithic catalyst material through proper choice of host and dopant atoms. This Phase I project will investigate the effects of certain additives to catalytically doped hexaaluminate ceramics for use in catalytic combustion. The catalytic dopants will include platinum and palladium while additives will include catalytically active transition metals and elements which are known to affect the activity of precious metal catalysts when used as substrates.

Selee Corporation
700 Shepherd Street
Hendersonville, NC 28792

57. Highly Efficient and Low Emissions Catalytic Radiant Burner

David Haack
704/697-2411

Funding Profile
Date Started: September 1, 1995

FY 95 - $75,000

The objective of this project is to develop catalytic foam radiant burners to replace existing radiant burners. In the past, porous radiant burner technology has been able to improve radiant energy output and reduce nitrogen oxide emissions below 15 ppm compared to conventional burners. Further improvements can be made by incorporating catalysts into the burners. Several catalytic radiant burners have been developed for various industrial applications (e.g., boilers and furnaces). Although the combustion performances of these burners are impressive, low lifetimes of combustion catalysts and burner substrates make them less attractive and keep them from being introduced to the market. Currently, several problems associated with existing catalytic radiant burners have been overcome by a unique foam radiant burner design. In this Phase I project, a new family of near-zero thermal expansion materials (e.g., sodium zirconium phosphates and their composites) will be used to prepare burner substrates. These burner substrates will be further coated with high temperature combustion catalysts. Foam radiant burners with various compositions and pore sizes will be fabricated. The effects of material composition and preparation process of porous foam on the combustion performance of the catalytic foam radiant burners will be examined.

Structured Materials Industrial, Inc.
120 Centennial Avenue
Piscataway, NJ 08854

58. Light Emitting Devices Based on Ge Quantum Crystals in a Direct Bandgap Matrix (AlN)

Gary S. Tompa
908/885-5909

Funding Profile
Date Started: September 1, 1995

FY 95 - $74,995

Recent observations of photoemission and absorption in nanoparticle material systems has strengthened the theory that the optical properties of nanocrystals can be drastically altered by quantum size effects. Such quantum effects have been demonstrated by observing white light electroluminescence and photoluminescence (from the infrared, through the visible, to the ultraviolet) in chemical-vapor-deposition-deposited thin films consisting of silicon (Si) and germanium (Ge) "quantum" crystals (QCs) embedded in a silicon dioxide matrix. Electroluminescent devices based on Ge QCs embedded in aluminum nitride (AlN) films will be developed in this project. These films will be formed by a unique ion beam assisted deposition process that has previously been used to deposit AlN films and shown to be compatible with large area processing. The advantage of the AlN host matrix over the SiO(2) host matrix system

is that the AlN can be doped n type and potentially p type. Therefore Ge QC electroluminescent devices containing p-n junctions in AlN-AlN or AlN-substrate structure can be fabricated, whereas p-n junctions cannot simply be fabricated with the SiO(2) host matrix films. It is expected that the direct bandgap and dopable AlN host matrix films will be an excellent alternative for high performance emitters and ultimately quantum crystal display applications. In Phase I, metal-insulator-semiconductor (MIS) structures will be fabricated using AlN films containing Ge QCs. Feasibility of the QC concept in this material system will be shown by demonstrating visible electroluminescent emission from AlN-based devices. The size and density of the Ge QCs will be controlled by the deposition parameters, as well as post deposition annealing. The bandgap of the QC is a function of the size: the smaller the size, the wider the bandgap. The wavelength of the visible emission can be adjusted by varying the QC size. Since Ge is an n-type dopant in AlN, the residual doping effects of the QC formation process will also be investigated, as well as possible effects associated with the nanocrystals. In Phase II, full color (white) electro-luminescent films for light-emitting diodes (LEDs) and displays based on MIS will be developed, and p-n junction devices will be fabricated from these QC films. A variety of LEDs and display products will evolve from this effort and be marked in Phase III.

TDA Research, Inc.
12345 West 52nd Avenue
Wheat Ridge, CO 80033

59. Low Cost, Novel Precursors to Beta" Alumina Solid Electrolyte

Ronald Cook
303/422-7819

Funding Profile
Date Started: September 1, 1995

FY 95 - $75,000

Advanced, high energy and high power density batteries, such as the sodium sulfur or the sodium metal chloride batteries, use beta" alumina, a fast sodium ion conductor, as the solid electrolyte. Unfortunately, the development and commercialization of these batteries has been hindered by problems with reliability of the beta" alumina. Conventional ceramic processing of beta" alumina is based on a solid state reaction between alpha alumina, Na(2)O, and Li(2)O, which requires high sintering temperatures and can lead to undesirable microstructures with poor mechanical properties. Improved processing that leads to a material with higher density higher fracture toughness, and improved control over grain size should improve the reliability of the beta" alumina. TDA Research, Inc. (TDA) has identified an improved, low-cost route to beta" alumina that has the potential to lower the sintering temperature, allow easier formability, and yield dense, high conductive polycrystalline material. In Phase I, TDA will prepare samples of beta" alumina through the new process in the form of disks and tubes, characterize the electrochemical properties and microstructure of the materials, and carry out an engineering analysis to compare the cost/performance of the new process to conventional methods.

Technology Assessment & Transfer, Inc.
133 Defense Highway
Suite 212
Annapolis, MD 21401

60. Nanolayer Coatings for Dry Machining: An Energy and Ecological Breakthrough Technology

David Crowther
301/261-8373

Funding Profile
Date Started: September 1, 1995

FY 95 - $74,761

Coatings capable of high-speed dry machining offer billions of dollars savings in energy and environmental costs. Pending OSHA and EPA legislation is increasing the pressure on industrial and government facilities to reduce the worker safety hazards of cutting fluids. This project will demonstrate the feasibility of magnetron sputtered coatings of novel material combinations and structures for dry machining. In Phase I, hard material systems with attractive high temperature properties will be deposited. Laboratory scale measurements of adhesion hardness, toughness, abrasion, friction, and wear, will precede coated insert turning tests. Feedback from property measurements and turning tests will provide guidance for compositional and processing coating refinements for specific classes of materials, such as cast iron, high alloy steels, aluminum and titanium.

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

61. A Low Emission AMTEC Automotive Power System

Thomas K. Hunt
313/677-4260

Funding Profile
Date Started: June 21, 1995

FY 95 - $331,248
FY 96 - $418,609

The alkali metal thermal to electric converter (AMTEC) is a static energy conversion device that operates at thermal to electric conversion efficiencies that are independent of size, have reached 19% efficiency, and are expected to reach 25% to 30% soon. These systems operate silently, with no moving parts and can utilize any source capable of delivering heat at 700 degrees C to 900 degrees C. Because they are efficient and small internal combustion engines with a wide range of output (within 5% of peak efficiency from 15% to 85% of full power), but use external combustion, they are expected to have the lowest emissions possible for a given electrical output. Their output is DC and, with appropriate series connection of modules, AMTEC can deliver voltages to match those provided by the battery systems of electric vehicles either for charging or for direct operation of electric motor drives. While AMTEC systems have been under development for years, recent advances made in programs directed toward spacecraft power systems have led to much simpler cell designs, far higher reliability, greatly improved modeling methods, and a clear path to modules appropriate for the assembly of multi-kilowatt systems. Phase I demonstrated an 18% efficient single-tube cell and the feasibility of producing, operating, and accurately modeling the experimental performance of multi-tube, series-connected AMTEC cells. In Phase II, a full-scale system design will be developed and used to guide experiments that allow a clear test of the feasibility of the AMTEC approach. A series of experimental cells will demonstrate the advanced component technologies required to reach 35% to 40% thermal efficiency, and the analytical models will then be used to determine the feasibility of a full-scale system. Phase II will conclude with an assessment of AMTEC utility for vehicle applications.

Advanced Refractory Technologies, Inc.
699 Hertel Avenue
Buffalo, NY 14207

62. Porous Aluminum Nitride Part Fabrication to Support Advanced Battery Development

Thomas J. Mroz, Jr.
716/875-4091

Funding Profile
Date Started: April 1, 1994

FY 94 - $599,703

In Phase I, sintered porous Aluminum Nitride (AlN) materials were shown to be suitable for separators in lithium-metal sulfide batteries. The sintered separator improves the structural integrity of the battery and allows reduction of the cell size. However, the current cost of AlN separators is more than the currently used Magnesium Oxide (MgO) powder materials. Methods of decreasing the cost of AlN separators have been identified - they involve reduction in powder cost, improvements in tape processing methods, and utilization of continuous firing methods. This project will investigate methods of obtaining these cost reductions through processing improvements. Additionally, extended battery testing will be performed to assist in separator plate optimization and to develop baseline characteristics for baseline development. Opportunities within the process have been identified that will provide suitable cost savings which would result in a cost competitive separator concept. Battery fabricators identified in Phase I will be used to evaluate these AlN separators in preparation for commercialization of the concept in Phase III. Other non-battery opportunities for the porous AlN structure have been identified which provide additional avenues for product commercialization.

American Superconductor Corporation
2 Technology Drive
Westborough, MA 01581

63. Oxide Dispersion Strengthened Silver for Use in High-Temperature Superconductor Composite Wires

Gilbert N. Riley, Jr.
508/836-4200

Funding Profile
Date Started: July 18, 1994

FY 94 - $125,000
FY 95 - $475,000

The strengthening of high-temperature superconductor (HTS) composite conductors with oxygen dispersion strengthened (ODS) silver is planned. State-of-the-art HTS composite conductors consist of ceramic superconductor filaments encased in a silver (Ag) sheath. For reasons of chemical compatibility and oxygen permeability, silver is the only material that can be used to sheathe HTS. However, the current method of manufacture weakens the silver sheath, resulting in reduced HTS conductor strengths. The low strength of these composite conductors is a major obstacle in the development of HTS wires for applications requiring robust conductors such as power transmission cables, SMES, and motors. ODS increases the strength of the sheath, while maintaining chemical compatibility and oxygen permeability of silver. In Phase I, two ODS-Ag systems and a method of fabrication were identified that provide the necessary thermomechanical stability and strength. Specific process issues unique to the materials and methods identified in Phase I will be addressed. Using insights gained from process-property-microstructure relationships and statistically designed experimental techniques, novel processes that simultaneously optimize the performance of the ODS-Ag sheath and the HTS will be developed. The resulting technology will be scaled up so that long lengths (approx. 1km) of high strength and high-performance HTS composite conductor can be manufactured on a routine basis.

Chemat Technology, Inc.
19365 Business Center Drive
Suite 8
Northridge, CA 91324

64. Capacitive Energy Storage Using High Surface Area Hafnium Compounds

Haixing Zheng
818/727/9786

Funding Profile
Date Started: July 18, 1994

FY 94 - $125,000
FY 95 - $475,000

High surface area materials have diverse applications, such as for energy storage systems and for catalytic converters. In Phase I, the feasibility of fabricating transition metal compounds with high surface area and high double layer capacitance, using the sol-gel process, has been demonstrated, and a supercapacitor cell has been prepared in the Phase I research. Several approaches have been tried to prepare these carbides, nitrides, and borides of high surface area with the focus on hafnium compounds which have the highest capacitance of >200 microfarad/cm(2). Hafnium carbonitrides with surface area up to 123 m(2)/g have been fabricated and the supercapacitor cell has been constructed using these porous hafnium carbonitrides. The cell has an energy density of 6.4 J/g, which is close to the 10 J/g energy density of ruthenium dioxide [RuO(2)]. In Phase II, energy storage capabilities will be enhanced by increasing the surface area of hafnium carbonitride and tailoring the chemistry of the pore surface. The best processing variables for fabricating the capacitive energy storage cells will be identified. The optimized cells will be tested for various properties: operation temperature, working voltage, capacitance, equivalence series resistance, and leakage current. All technical parameters will be measured and a technical database on these supercapacitors will be prepared for future commercialization of the supercapacitors. The process will be scaled up to pilot plant stage, and the production cost will be estimated.

EIC Laboratories, Inc.
111 Downey Street
Norwood, MA 02062

65. Economical Photochromic Films Based On Metal Oxides

R. David Rauh
617/769-9430

Funding Profile
Date Started: June 21, 1995

FY 95 - $249,250
FY 96 - $487,470

The goal of this work is to develop a robust thin film coating, less than two microns thick, that can be applied to surfaces, rendering them photochromic in sunlight with respect to both the visible and near infrared components of the solar spectrum. Computer models have anticipated that photochromic windows would give rise to significant energy savings by solar management, particularly in buildings dominated by their cooling load. The proposed coatings are derived from thin film transition metal oxides and are expected to be economical in materials and preparation, robust, and insensitive to environmental degradation. The objective of Phase I was to demonstrate a new highly active metal oxide film employing a novel means of sensitization. The photocoloration rate of tungsten oxide was increased 16-fold using this approach and the final optical density by a factor of three. The best Phase I films showed photocoloration under simulated solar conditions from 0.8 to 0.3 luminous transmittance with a coloration time of about 30 minutes, sufficient for energy control applications. However, bleaching times in air exceeded 24 hours and the dynamic range degraded after a few cycles. The objective of Phase II is to further improve the technology to achieve films with similar dynamic coloration properties but with bleaching rates in the dark of about 30 minutes and greater than one thousand cycles without loss of dynamic range. The Phase II research and development will focus on the reversibility of the sensitization process along with film fabrication methods applicable to the incorporation of a variety of possible sensitizer materials, extending approaches initiated in Phase I. Phase II will also develop a process for deposition onto polymer substrates used in window control films. Analyses of manufacturing costs and of solar energy transfer through windows incorporating photochromic films will also be carried out, permitting a final estimate of energy payback in various climates.

ISM Technologies, Inc.
9965 Carroll Canyon Road
San Diego, CA 92131

66. Low Temperature Deposition of Titanium Nitride

Anthony J. Perry
619/530-2332

Funding Profile
Date Started: July 18, 1994

FY 94 - $124,933
FY 95 - $474,744

Titanium Nitride (TiN) has been found to be an excellent coating for wear resistant applications. However, the deposition temperature of about 450 degrees C is far too high for many applications for machine component parts made from alloy steels or aluminum alloys, where deposition temperatures over 150 degrees C would deleteriously affect the mechanical properties of the substrates. When TiN coatings deposited at such a temperature, using current conventional industrial technologies, the micro-structure is not dense and the resulting coatings have mechanical properties far inferior to those made at the higher temperatures. Phase I demonstrated that hard, well-adhering TiN with low residual stress and a dense micro-structure can indeed be made at 150 degrees C (by reactive deposition from a cathodic arc evaporation source) using the Hyper-Ion process developed by ISM Technologies. In the Hyper-Ion process, a pulsed high voltage bias is applied to the work-piece which produces this marked improvement in properties. In Phase II, the deposition process should be further developed and refined to produce a well-defined coating process, which can be scaled up into production, aimed at providing optimized wear resistance industrial parts.

JX Crystals Inc.
1105 12th Avenue, NW
Suite A-2
Issaquah, WA 98027-8994

67. A Clean and Efficient Thermophotovoltaic Generator for Electric Vehicles

Lewis M. Fraas
206/392-5237

Funding Profile
Date Started: June 21, 1995

FY 95 - $253,675
FY 96 - $496,322

This project is developing thermophotovoltaic energy systems to address several problems with conventional small electric generators. Conventional internal combustion models are widely used in the commercial and military sectors for remote, back-up, and portable power. Existing problems include low fuel efficiency, high maintenance, emissions, and noise. Using a thermophotovoltaic energy system to cogenerate electricity and heat, all of these problems can be addressed. In Phase I, a thermophotovoltaic demonstration unit was developed. This proved the concept of generating electricity by surrounding an emitter radiating in the infrared with infrared-sensitive photovoltaic cells. With a fan as the only moving part, this clearly demonstrated low noise and the potential for low maintenance. By maintaining a constant burn temperature, emissions were much lower than those from a periodically exploding internal combustion engine. Finally, the potential for high efficiency by using the waste heat for space and water heating is evident, and achieving the cost and size of existing generators appears feasible. The planned effort for Phase II is the optimization of key components, development of a one kilowatt cogenerator, and the installation of a thermophotovoltaic system into an existing electric car. The Phase II effort provides valuable component optimization and another iteration of generator development for this electric vehicle effort, as well as taking the natural step of installing the multi-kilowatt generator in a car. More importantly, Phase II will provide a full-scale demonstration of the cogeneration technology.

Selee Corporation
700 Shepard Street
Hendersonville, NC 28792

68. High Strength Ceria-Zirconia Toughened Alumina Ceramic with Superior High Temperature Strength and Corrosion Resistance

Giulio A. Rossi
704/697-2411

Funding Profile
Date Started: June 21, 1995

FY 95 - $145,398
FY 96 - $279,767

This project deals with the development of a novel ceramic material with superior strength and corrosion and erosion resistance in high-temperature environments. This material was shown to exhibit strength and thermal shock resistance superior to that of alumina and mullite. Phase I showed it to have excellent resistance to high temperature sulfates and alkalies, though the tests were not of long enough duration to demonstrate this conclusively. In Phase II, samples of open celled ceramic foam will be fabricated by impregnation of a polyurethane foam with an aqueous ceramic slurry followed by drying and firing to burn out organic material and densify the foam struts at high temperature. Several variables will be studied including zirconia/alumina ratio, particle size and several processing variables. The samples will be physically characterized. High-temperature cycling will also be done using a gas burner rig. Degradation of modulus of elasticity as the result of thermal cycling will be carried out. Samples will also be exposed to high temperature and pressure in atmospheres typical of the integrated gasification combined cycle and pressurized fluid bed combustor coal burning processes. The exposed samples will be examined for evidence of chemical attack.

Space Power, Inc.
621 River Oaks Parkway
San Jose, CA 95134

69. Design and Applications of Close-Spaced Thermionic Converters with Novel Isothermal Electrodes

Gary O. Fitzpatrick
408/434-9500

Funding Profile
Date Started: June 21, 1995

FY 95 - $253,676
FY 96 - $496,324

Thermionic converters with close-spaced interelectrode gaps are capable of substantial performance improvements over conventional ignited mode diodes. At very close gaps (two to 10 microns), a thermionic converter operates in the collisionless Knudsen mode with nearly double the output voltage of conventional diodes and concomitant increases of efficiency. In Phase I, a special electrode structure that can accommodate high heat flux without distortion was investigated. This type of electrode is needed in order to maintain an interelectrode gap of about five microns and to avoid short circuiting by thermal expansion deformation. In Phase I, a laser interferometric technique was also developed to measure the thermal expansion deformation of electrodes with high heat fluxes passing through them. In Phase II, the electrode investigation is further extended with new features to increase power density and higher operating temperatures. The higher power density operation is attractive for utility topping cycles and cogeneration. Additional experiments using laser interferometry will be carried out in Phase II and complete thermionic converters with novel features to produce substantially increased efficiency and power density will be tested. Prototypic devices with silicon carbide hot shells will be constructed and operated in an effort to develop a practical diode for commercial applications. Although electrical heat sources will be used for experimentation in Phase II, the type of converters that will be built would be suitable for operation with flame heat sources or solar concentrators operating in atmospheric air.

Thermal Electric Devices, Inc.
1704 Stanford Dr. NE
Albuquerque, NM 87106

70. Development of Metal Hydride Materials for High Coefficient of Performance Heat Pumps

K. Thomas Feldman, Jr.
505/268-0154

Funding Profile
Date Started: March 11, 1995

FY 95 - $375,000
FY 96 - $375,000

An efficient hydride reactor is necessary to allow an environmentally clean hydride heat pump to achieve its potential to be twice as efficient as current systems. A practical and cost effective method of coating hydride particles with high thermal conductivity copper and then compressing and sintering them into porous powder metal hydride (PMH) compacts with improved heat transfer was developed in Phase I. Thermal conductivity, k = 7.5 W/(m.degrees C) was measured on green PMH compact pellets, a factor of 18 better than that of uncoated hydride particles. Transient analysis of reactor performance with a numerical code indicates only k = 5 W/(m.degrees C) is required to achieve an adequate heat transfer rate for the heat pump. Further optimization of the PMH compacts is needed to improve thermal conductivity to 10 W/(m.degrees C) which will provide excellent heat pump performance. Phase I results are highly promising. Phase II will further develop the PMH compacts into the shape of disks that can be press fit into a hydride reactor. The PMH compact disks will have grooves to improve hydrogen flow and will have thermal conductivity of at least 10 W/(m.degrees C). PMH compact disks with embedded high thermal conductivity fibers will be explored as composite structures with high thermal conductivity and strength. Hydride reactors with these PMH compact disks will be built and tested for thermal performance. The numerical analysis code for heat-driven hydride reactors will be rewritten to describe the more promising compressor-driven hydride heat pump. The performance of the hydride heat pump, including electric energy consumption, cooling rate, coefficient of performance, weight, volume, cost, and life cycle cost, will be predicted and compared both with the experimental test data and with performance data of conventional vapor compression systems.

Ultramet
12173 Montague Street
Pacoima CA 91331

71. Coated Micrograin Carbides for Wear Resistance

Andrew J. Sherman
818/899-0236

Funding Profile
Date Started: July 18, 1994

FY 94 - $124,908
FY 95 - $474,649

Micrograin carbides are small grain size (1-5 micron diameter) particles of tungsten carbide (WC) that have been "cemented" together with a predominantly cobalt matrix by liquid-phase sintering. The result is an excellent material for carbide cutting tools and other wear- and/or corrosion-resistant parts, because their finer grain size yields better mechanical properties than typical carbide tools (with grain sizes 20-50 micron). Some of their potential advantage is negated, however, by the difficulty of handling such fine powders and mixing them with cobalt powders to form the blend which is then preformed and sintered. Problems arising during handling and blending include increased impurity content, nonhomogeneous distribution of matrix powders, and WC-WC particle contact, all of which lower mechanical properties in the finished part. Also, substantial grain growth occurs during the liquid-phase sintering step. The result is that cobalt content must be increased to achieve the desired fracture toughness and transverse rupture strength, with a corresponding decrease in tool hardness and life and an increase in tool cost. In Phase I, the feasibility of coating individual WC grains with the proper thickness of cobalt matrix was demonstrated. After consolidation, the problems of WC-WC particle contact and mixed carbide formation were found to be eliminated. Improved mechanical properties and performance over conventional micrograin carbides were obtained. The process permitted faster consolidation times and yielded lower impurity content with less deleterious interaction between matrix and carbide, as well as a large reduction in the amount of cobalt required. In Phase II, the process for coating WC/mixed carbide powders with cobalt will be optimized. A 40% increase in tool life (reduced wear rate) at constant mechanical properties and lower cobalt content, and/or a 50% increase in tool toughness (and hence strength) at constant wear is expected.

APPENDIX A

PROGRAM DATA

OFFICE OF COMPUTATIONAL AND TECHNOLOGY RESEARCH

ADVANCED ENERGY PROJECTS DIVISION

BUDGET

	FY 1994	FY 1995	FY 1996 (REQUEST)
OPERATING	$11,400,000	$11,085,000	$12,026,000
EQUIPMENT	300,000	242,000	300,000

DISTRIBUTION OF FY 1995 FUNDS

Universities	46%
DOE Laboratories	50%
Other	4%

INVESTIGATOR INDEX
(Project Numbers)

Anders, Simone	17
Bardsley, J. N.	19
Benson, David K.	28
Besmann, Theodore M.	33
Bionta, Richard M.	20
Bromberg, Leslie	26
Cook, Ronald	59
Crowther David	60
Dowben, Peter A.	32
Farmer, Joseph C.	21
Feldman, K. Thomas	70
Fitzpatrick, Gary O.	69
Fraas, Lewis M.	67
Gourley, Paul	36
Greene, Philip	38
Gruen, Dieter M.	4
Gschneidner, Jr., Karl A.	2
Haack, David	57
Hanna, Mark C.	29
Hertzberg, Abraham	43
Ho, Kai-Ming	3
Huffman, Donald R.	7
Hunt, Thomas K.	61
Jeng, King Tsai	52
Jensen, Reed J.	23
Joshi, Chan J.	10
Kapteyn, Henry C.	45
Kazmerski, Lawrence L.	30
Liu, Paul K.T.	53
Mattick, Arthur T.	44
Michl, Josef	13
Mroz, Jr., Thomas J.	62
Nastasi, Michael	24
Nebel, Richard A.	25
Nozik, Arthur J.	31
Pantell, Richard H.	39
Pekala, Richard W.	22
Perry, Anthony J.	66
Pfefferle, William	56
Putterman, Seth J.	11
Rabitz, Herschel	34
Rauh, R. David	65
Riley, Jr., Gilbert N.	63
Robinson, J. Michael	42
Rose, M. Frank	8
Rosen, Moshe	16
Rossi, Giulio A.	68
Rubin, Michael D.	18
Ryu, Jaeseok	47
Schuessler, Hans A.	41
Seal, Michael R.	46
Sherman, Andrew J.	71
Skelly, David W.	15
Smith, Paul	12
Stangle, Gregory C.	1
Stinnett, Regan W.	37
Swette, Larry L.	49
Temkin, Henryk	14
Testardi, Louis R.	40
Tomczuk, Zygmunt	5
Tomkiewicz, Micha	9
Tompa, Gary S.	58
Treglio James R.	51
Tsao, George T.	35
Warren, David	50
Was, Gary S.	27
Weaver, Samuel C.	54
Weimer, Raymond J.	48
Wiederrecht, Gary P.	6
Yadav, Tapesh	55
Zheng, Haixing	64

INSTITUTIONAL INDEX
(Project Numbers)

Advanced Modular Power Systems, Inc.	61
Advanced Refractory Technologies, Inc.	62
Alfred University	1
American Superconductor Corporation	63
Ames Laboratory	2, 3
Argonne National Laboratory	4, 5, 6
Arizona, University of	7
Aspen Systems, Inc.	47
Auburn University	8
Brooklyn College of City University of New York	9
California, University of, Los Angeles	10, 11
California, University of, Santa Barbara	12
Chemat Technology, Inc.	64
Colorado, University of	13
Colorado State University	14
Cordec Corporation	48
EIC Laboratories, Inc.	65
General Electric Company	15
Giner, Inc.	49
Harvest Technology	50
ISM Technologies, Inc.	51, 66
Johns Hopkins University	16
JX Crystals, Inc.	67
Lawrence Berkeley Laboratory	17, 18
Lawrence Livermore National Laboratory	19, 20, 21, 22
Los Alamos National Laboratory	23, 24, 25
Lynntech, Inc.	52
Massachusetts Institute of Technology	26
Media and Process Technology, Inc.	53
Michigan, University of	27
Millennium Materials, Inc.	54
Nanomaterials Research Corporation	55
National Renewable Energy Laboratory	28, 29, 30, 31
Nebraska, University of	32
Oak Ridge National Laboratory	33
Precision Combustion, Inc.	56
Princeton University	34
Purdue University	35
Sandia National Laboratories, Albuquerque	36, 37
Science Research Laboratory	38
Selee Corporation	57, 68
Space Power, Inc.	69
Stanford University	39
Structured Materials Industrial, Inc.	58
TDA Research, Inc.	59
Technology Assessment & Transfer, Inc.	60
TecOne	40
Texas A&M University	41
Texas, University of	42
Thermal Electric Devices, Inc.	70
Ultramet	71

INSTITUTIONAL INDEX, Cont'd.
(Project Numbers)

Washington, University of	**43, 44**
Washington State University	**45**
Western Washington University	**46**

APPENDIX D

FACSIMILE COVER SHEET

DATE: _____

TO: **Advanced Energy Projects Division**
ER-33, GTN
U.S. Department of Energy
19901 Germantown Road
Germantown, MD 20874-1290

FROM: _____
(inc. tel #)

_____

SIGNATURE: _____

_____	**M. H. Bhattacharyya**	_____	**G. C. Carter**
_____	**W. M. Polansky**	_____	**S. E. Stottlemyer**

Message:

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