Chapter 3
Clean and Affordable Power

Scientific Challenge: ***To understand the physical, material, and chemical processes for advanced power generation, storage, and transmission.***

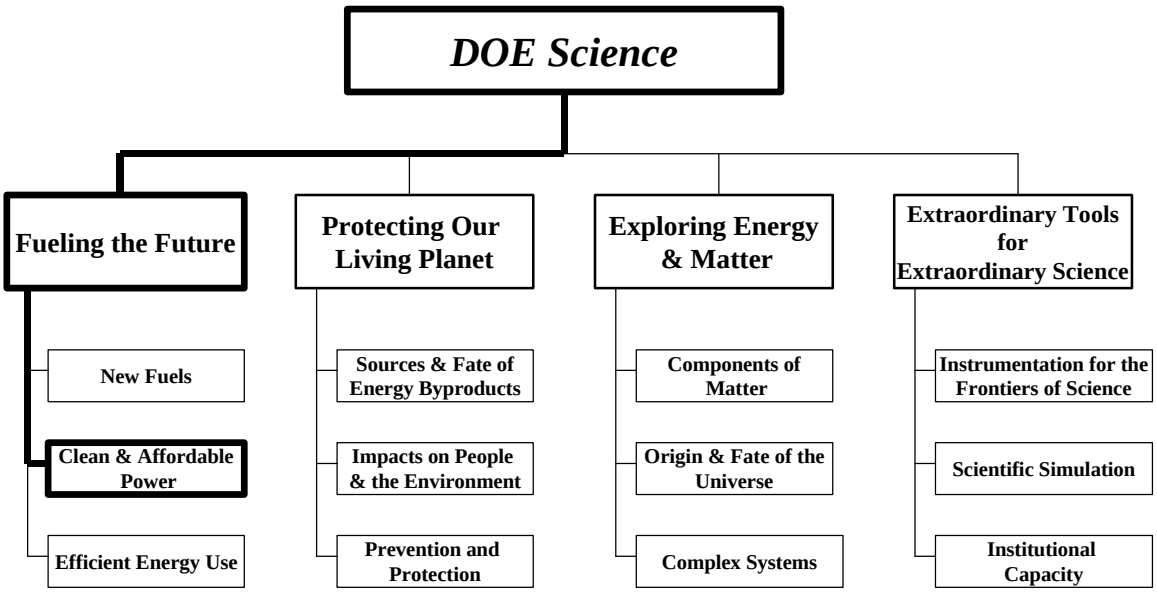

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Table of Contents

Page

Plasma Science and Fusion Research 31
Description, Objectives, and Research Performers 31
Research Challenges and Opportunities 31
Research Activities 32
Accomplishments 32

Condensed Matter Physics 33
Description, Objectives, and Research Performers 33
Research Challenges and Opportunities 33
Research Activities 34
Accomplishments 34

Metal and Ceramic Sciences 35
Description, Objectives, and Research Performers 35
Research Challenges and Opportunities 35
Research Activities 36
Accomplishments 37

Energy Production, Storage, and Transmission 37
Description, Objectives, and Research Performers 37
Research Challenges and Opportunities 38
Research Activities 38
Accomplishments 38

Portfolio Summary 39

New and continued advancements in our scientific knowledge will provide the nation with power that is economically competitive while meeting environmental standards. Clean and affordable power has two focus areas: (1) advanced power systems and (2) enhanced electric utility infrastructure.

The advanced power systems area includes plasma science and all aspects of nuclear fusion. Plasma science is an important element of the scientific infrastructure of the country, and fusion energy is the “grand challenge” of plasma science. Although most of the visible matter in the universe is in the plasma state, plasmas are rare on earth and can only be studied in complex laboratory experiments. This is a long-term research and development program with huge potential impact on both advanced power systems and infrastructure in the middle to later part of the next century.

The utility infrastructure focus area is associated predominantly with the basic and fundamental science needed for efficient conversion of chemical and mechanical energy to electric energy, efficient distribution, and final utilization of electrical energy. Research underway that will impact the energy infrastructure of the future includes condensed matter physics underlying superconductivity and transport properties of matter, the engineering of advanced materials for hardness and mechanical stability, materials design for radiation resistance, research on magnetic materials, fundamental understanding of the mechanical behavior of materials, and design of new materials.

Plasma Science and Fusion Research

Description, Objectives, and Research Performers

The process of nuclear fusion - evident in stars, including the Sun - releases enormous amounts of energy. The three goals of the program are to advance plasma science, develop fusion science and concept innovation, and pursue fusion energy as an international collaboration. The mission is to advance the knowledge base needed to make fusion an economically and environmentally attractive power source for the future. This research is conducted at national laboratories, universities, and industrial firms.

Research Challenges and Opportunities

Although the burning of fusion fuels (deuterium and tritium) does not produce radioactivity, the tritium itself is radioactive, and the neutrons produced by fusion will induce radioactivity in surrounding materials. Although fusion has great potential as a safe and environmentally benign source of energy, there are safety and environmental issues associated with radioactive materials in future fusion devices; these issues will need to be addressed. Tritium handling, which has a strong influence on these issues, requires technologies that are significantly advanced from today's capabilities for control, containment, and processing of tritium in the large quantities expected for future fusion devices. Developing an attractive fusion energy source requires major advances in technologies for plasma and neutron-interactive fusion power core components and in neutron-interactive structural materials with the potential for superior performance in fusion energy systems. The hostile neutron irradiation environment of future fusion power cores will place unprecedented demands on structural materials.

There are two promising approaches to achieving fusion energy: magnetic and inertial confinement. Theory and simulation of plasma behavior in both magnetic and inertial fusion is complex because of the many orders of magnitude in spatial and temporal scales involved. It is further complicated by the need to understand electromagnetic wave/plasma interactions and plasma material interactions.

The long-term potential for successful commercialization of fusion energy could radically change the overall pattern of electricity generation. Because fusion power plants would not produce air pollutants that contribute to acid rain and that may contribute to global climate change, they could minimize the environmental risks associated with the burning of fossil fuels. Further, because fusion power plants would contain only small quantities of fuel at any time, they could eliminate the potential for runaway reactions that might lead to accidents. The development of low-activation materials or advanced fuel cycles for fusion reactors could make the amounts of high-level radioactive waste that result from fusion-produced energy far smaller than those produced by fission reactors—thus simplifying waste disposal problems. The experimental program with heavy ion drivers shows promise for significantly advancing inertial fusion science.

Research Activities

Theoretical and computational research in plasma science provides the predictive capability needed to make progress in plasma and fusion science. Current research areas include plasma turbulence and its effect on the transport of particles and energy in plasmas, macroscopic equilibrium and stability of confined plasmas, edge plasma physics and plasma material interactions, plasma heating and current drive with radio-frequency waves, and understanding the characteristics of innovative confinement configurations. Plasma theory and simulation are also key to understanding other scientific phenomena, such as magnetic reconnection in solar and magnetospheric plasmas or turbulence, chaos, and self-organized behavior in complex systems. Finally, simulation in plasma physics is similar to and promotes progress in fields such as computational fluid dynamics and climate modeling.

The plasma technologies program provides the technology tools needed to create, control, and understand the high-temperature plasma state in fusion experiments. Experiments on the DIII-D and Alcator C-Mod tokamaks are being carried out in combination with continuing theoretical development to dramatically reduce energy losses in these experimental fusion energy systems. An important new facility, the National Spherical Torus (NSTX) will begin operations in FY 1999. This proof-of-principle level facility will investigate the physics of the promising spherical torus concept. Collaborative experiments with our major international partners will also attempt to scale these results to energy producing plasmas.

Accomplishments

- Significant progress has been made in understanding the behavior of magnetically confined plasmas during the past 10 years. Three-dimensional simulations of microturbulence and the associated energy transport in tokamaks, including the effects of turbulence suppression by zonal flows, agree well with analytic calculations and

qualitatively with experimental results. Similar calculations have been carried out for the edge plasma region, and the physics of edge transport barriers is fairly well described.

- Equilibrium and stability calculations combined with current and pressure profile control calculations have identified advanced tokamak operating regimes that are now being explored experimentally. Predictions of instabilities driven by the fusion-produced, alpha particles in a tokamak have been verified in the Tokamak Fusion Test Reactor (TFTR) and the Joint European Torus (JET).

- Credible models of the plasma boundary/divertor regions of a tokamak plasma have been developed, and extrapolations to burning plasma devices are becoming increasingly reliable. These accomplishments in understanding the behavior of magnetically confined plasmas put scientists one step closer to developing an economically and environmentally attractive fusion energy source.

- Extensive new computational tools to help with the design of alternative fusion confinement configurations, particularly stellarators, have been developed and applied to the design of a new generation of small-scale experiments.

- The heavy ion driver single beam, multiple beam and focusing experiments are demonstrating the scientific basis for induction accelerators in the fusion science program.

Condensed Matter Physics

Description, Objectives, and Research Performers

Research in condensed matter physics is aimed at gaining a fundamental understanding of the behavior of materials. Experimental measurements seek to determine electronic structure, transport properties, phase transitions, mechanism for high temperature superconductivity, complexity in electronic interactions, and self-organization of electronic states. This includes fundamental measurements of the properties of solids, liquids, glasses, surfaces, thin films, artificially structured materials, self-organized structures, and nanoscale structures. This activity also supports basic research in theory and simulations of condensed matter, the use of ion beams to study and modify the properties of materials, and engineering applications. The theory activity complements much of the experimental work by guiding, stimulating, and explaining experiments. It includes the support of selected centers with specific materials-related missions. These centers excel in bringing together individual scientists from widely different backgrounds to work on common research areas or make use of common research tools. Included among these are the Center for X-ray Optics and the Centers for Advanced Materials at Lawrence Berkeley National Laboratory and the Surface Modification and Characterization Facility at Oak Ridge National Laboratory. This research is conducted at national laboratories and universities.

Research Challenges and Opportunities

The major unresolved research question in condensed matter physics is the physical mechanism that makes high temperature superconductivity possible. Another issue relates to giant or

colossal magnetoresistance. A major challenge is the theoretical understanding of high temperature superconductivity, and of the electronic structure and properties of complex, multicomponent materials.

Future efforts will include continued support for investigations of materials with increasingly complex behavior, composition and structures with strongly competing interactions among the electronic charge and spin, and the crystalline lattice. A major new activity will be the synthesis and fabrication of unusual materials systems with pulsed laser ablation epitaxy, self-organized structures, and engineered materials and structures to provide insight into unusual behavior.

Research Activities

The materials examined include magnetic materials, superconductors, semiconductors and photovoltaics, liquid metals and alloys, and complex fluids. The measurements include optical and laser spectroscopy, photoemission spectroscopy, electrical and thermal transport, thermodynamic and phase transition measurements, nuclear magnetic resonance, and scanning-tunneling and atomic-force microscopies. The development of new techniques and instruments, including magnetic force microscopy, electron microscopic techniques, and innovative applications of laser spectroscopy, are major components of this activity. Measurements will be made under extreme conditions of temperature, pressure and magnetic field.

The program supports items such as lasers, scanning-tunneling microscopes, electron detectors for photoemission experiments, sample chambers, superconducting magnets and computers. Activities include the design and construction of new, unique research instruments, such as the 100 Tesla Pulsed Field Magnet and the actinide photoelectron spectrometer at Los Alamos National Laboratory.

The emphasis in engineering physics is on the use of fundamental science to advance technology. Engineering physics includes activities such as the application of sound waves for refrigeration; the fabrication of small, machined structures using x-rays; and the development of new, electron microscopy techniques such as the Z-contrast electron microscope at Oak Ridge National Laboratory.

Accomplishments

- First proof of a thermodynamic first-order transition from a solid-like vortex lattice to a vortex liquid in a high-temperature superconductor is leading to development of a new state of matter called vortex matter. The nature of this transition is significant for fundamental theories of phase transitions and for practical applications of superconductivity. For example, movement of the vortices in response to an electric current dissipates the energy of the current—the resistivity is not zero—and the material is not superconducting.

- Improvements in our knowledge of behavior of condensed matter physics have been applied to develop photovoltaic solar cells that convert sunlight into electricity with 30% efficiency—far greater than the 10-20% efficiencies of earlier devices.

- The discovery of a new electrolyte system, lithium phosphorus oxynitride, which is stable in contact with lithium metal, has enabled the development of thin-film batteries approximately 10 microns thick which have unsurpassed energy densities and can operate safely at temperatures as high as 150 degrees C.

- It was discovered that when nickel is cold rolled into a thin film of superconducting material, the crystalline grains tend to line up and produce oriented films, which allows relatively long lengths of HiTc conducting tape to carry substantial amounts of electric current.

- A novel surface diffusion process first predicted by theory was verified by electron microscopy and has become an important consideration in all modern treatments of surface diffusion. Surface diffusion plays a key role in phenomena such as crystal growth, thin film stability, and chemical reactions.

- Certain three dimensional periodic structures have been shown to possess a photonic bandgap, i.e., a frequency region where the propagation of electromagnetic waves is forbidden for all wave lengths. These structures show promise as antennas, resonant filters, and detectors. This photonic effect results from the contrast in the dielectric properties between the material and air, and is an example of how geometry can play a powerful role in the behavior of materials.

- Quantum mechanical calculations have led to the prediction of the existence and properties of yet unknown materials, e.g., C3N4, which rival diamond in hardness. If efforts to synthesize these materials are successful, they would provide options for new coatings, abrasives, and cutting tools.

Metal and Ceramic Sciences

Description, Objectives, and Research Performers

This activity supports fundamental experimental research that specifically targets the needs of the DOE technology programs and, therefore, has significant impacts on energy generation, transmission, conversion, and conservation technologies. The work conducted in this program is long-term fundamental research in materials, with a focus on the influence of synthesis and processing on the materials' structure and properties. Mechanical behavior and radiation damage are also studied to understand the fundamental principles of the defect-property relationship on an atomic level, so that predictive models can be developed that will permit the design of materials that have desired mechanical behavior and resistance to irradiation damage. Linkage of materials' structure at the atomic level to behavior at the continuum level will become a reality, thus bringing new rigor to the science of mechanical behavior. This research is conducted predominantly at national laboratories and universities.

Research Challenges and Opportunities

Many critical unresolved issues concern the mechanical behavior of materials that have been with us for a long time, but have not been subjected to contemporary multidisciplinary

investigation. As in other areas of materials science, recent developments in diagnostics and computation are enabling researchers in mechanical behavior to probe regimes that had not previously been accessible to them. Real time *in-situ* diagnostics now available with programmed mechanical behavior response measurements permit the observation of the evolution of the structure of materials during deformation. The computational capabilities of massively parallel processors allow the simulation of multiple simultaneous processes at different lengths of scale, thus providing a new opportunity for fundamental discovery of deformation mechanisms. Intense and tunable X-ray beams and small angle scattering capabilities also offer myriad opportunities for the in-situ characterization of deformation mechanisms. The challenge is to synthesize these new insights into mechanistically rigorous, validated, predictive models.

The impact is clear—mechanical behavior and radiation effects phenomena underpin the structural reliability and safety of energy generation, conversion, transmission, and conservation systems. Mechanical and irradiation-induced failures may lead to, for example, the escape of undesirable fluids or gases into the environment. In an age when economy necessitates life extension, the ability to predict performance reliably (from a fundamental basis) is becoming key.

Research Activities

Activities include the synthesis and processing of materials with new or improved behavior and/or with reduced waste byproducts; hard and wear-resistant surfaces to reduce friction and wear; high-rate, superplastic forming of lightweight, metallic alloys for fuel-efficient vehicles; and high-temperature structural ceramics and ceramic matrix composites for high-speed cutting tools and fuel-efficient and low-pollutant engines. Quantitative, non-destructive analysis provides early warning of impending failure, prediction of remaining reliable service life, and on-line, in-situ flaw detection during fabrication or production. Response of magnetic materials to applied static and cyclical stress is investigated. Research into plasma, laser, and charged particle beam surface modification should yield increased corrosion or wear resistance. Another research area involves processing of high-temperature, high-strength yet fabricable intermetallic alloys; and welding and joining of alloys, ceramics, and dissimilar materials.

Mechanical behavior activities include investigations of deformation and fracture mechanisms, mechanical load-bearing ability, failure and cyclic fatigue resistance, stress-corrosion, high strain-rate behavior, fracture toughness and impact resistance, high-temperature strength, creep-fracture and dimensional stability, and deformation behavior and formability. Radiation effects activities include investigations of mechanisms of neutron irradiation damage and ion implantation into solid surfaces, modeling, predicting and controlling neutron radiation damage, irradiation-assisted stress corrosion cracking, and surface modification by ion implantation. Significant research that brings together basic and applied researchers takes place under the distributed Center of Excellence for the Synthesis and Processing of Advanced Materials.

Accomplishments

- A new model for electrical resistance spot welding utilizes a unique incrementally coupled finite element modeling approach that takes appropriate account of the deformation and consequential change in the shape of welding electrode contact surfaces.

- Stronger and cheaper magnets have been produced by adding titanium and carbon to a molten neodymium-iron-boron alloy, which permits a spray atomization process to produce nanocrystalline composite powder with a crystallite size that matches that of the magnetic domains in this alloy, which in turn causes this material to produce stronger and cheaper magnets.

- A uniform three-dimensional coating process known as plasma immersion ion processing has been developed. It results in the production of hard coatings, such as diamond-like carbon, that exhibit low sliding-friction and superior wear resistance. Coatings produced by this process may easily be scaled to large areas (many square meters), are uniform over irregular surfaces, produce adherent coatings on a wide variety of substrates, and are economical.

- Research demonstrated that commercially important self-reinforced silicon nitride ceramics must be tailored at the microscopic and atomic levels. This resulted in the formation of low aluminum and oxygen surface layers which in turn yielded an exceptionally high fracture resistance in this ceramic.

- Combining surface-sensitive synchrotron X-ray diffraction with in-situ real-time electrochemical experiments revealed the surprising discovery that the passive oxide that forms on pure iron or on stainless steel has a very fine-grained “nanocrystalline” structure. This startling conclusion overturns the long accepted belief that stainless steel is corrosion resistant because the passive film was thought to be non-crystalline.

Energy Production, Storage and Transmission

Description, Objectives, and Research Performers

This activity addresses energy aspects of chemically related engineering sciences, including thermodynamics, turbulence related to combustion, and physical and chemical rate processes. Particular attention is given to experimental and theoretical aspects of phase equilibria, especially of mixtures, including supercritical phenomena, and to the physics of gas phase turbulence. Also included are fundamental studies of thermophysical and thermochemical properties. Emphasis is given to improving and/or developing the scientific base for engineering generalizations and their unifying theories. Also included is fundamental research in areas critical to understanding the underlying limitations in the performance of electrochemical energy storage and conversion systems. Areas of research include the characterization of anode, cathode, and electrolyte systems and their interactions. The program covers a broad spectrum of research, including fundamental studies of composite electrode structures, failure and degradation of active electrode materials, and thin film electrodes, electrolytes, and interfaces.

The aim is providing knowledge that will lead to improvements in battery size, weight, life, and recharge cycles.

Research Challenges and Opportunities

A major challenge is to understand the fundamental chemical engineering sciences that underpin nearly all energy intensive chemical processes. In this regard, particular emphasis is placed on electrochemical storage and conversion, and turbulence both in combustion and in fluid flow. New opportunities have been identified associated with the need to couple the current emphasis of the program in molecular simulations with molecular level theory. This new knowledge will reduce the uncertainty in calculations and provide a better molecular-level basis for engineering generalizations and theoretical tools. Development of a molecular-level understanding of the physical and chemical processes is important to the environmentally benign utilization and conversion of our fossil energy resources.

Research Activities

Fundamental research in energy aspects of chemically related engineering topics using advances in molecular and statistical mechanics, quantum chemistry, and molecular simulation emphasizes improving and/or developing the scientific base for engineering generalizations and their unifying theories. Fundamental research critical to understanding the underlying limitations in the performance of electrochemical energy storage and conversion systems focuses on the study of the electrochemical interactions of electrochemical couples and electrolytes at heterogeneous and buried interfaces. Although the focus of the Office of Science research is on non-automotive electrochemical energy storage and conversion systems, the fundamental knowledge gained may have broad application.

Accomplishments

- Fundamental research in the deposition of reactive metals and their mobility and stability in non-aqueous electrolytes identified those organic electrolytes that led to the development of the current generation of high energy and power lithium and lithium ion batteries. Because of their performance advantages, they are now widely used in consumer and defense applications and are under further development for use in electric vehicles.

- Research has resulted in a new solid polymer electrolyte system that exhibits high room temperature conductivity. This advance resulted from the ability to minimize the strength of the interaction between the lithium complex and the polymer network by controlling the void volume of the network and the hydrophobicity of the interface.

- Fundamental research in ion transport in glassy solids has led to the successful development of thin film lithium battery technology, producing batteries half the thickness of household plastic wrap.

- Basic research in non-aqueous liquid electrolyte systems has led to an approach for prevention of the oxidation of alkali metal electrodes by the electrolyte. This has led to

the development of a non-flammable organic liquid electrolyte for lithium and lithium ion battery systems; the modified electrolyte has improved the safety of rechargeable batteries.

Portfolio Summary

This portfolio area, "Clean and Affordable Power," encompasses research from many programs and supporting activities that crosscut the research topics covered above. The table below summarizes specific programs that strongly support or moderately support clean and affordable power, including plasma science and fusion research; condensed matter physics; metal and ceramic sciences; and energy production, storage, and transmission. The funding totals for these areas are an analytic tool reflecting the highly crosscutting, leveraged aspects and implications for individual research areas within DOE's science portfolio. **Because research areas may appear in multiple chapters, there will be significant instances of multiple counting, and the chapter totals will not sum to the overall science budget.** Additional details on these research areas are presented in the Research Summary Matrix and the corresponding Research Summary Profiles.

Strongly Supportive RSPs (Combined Budget: $393.86 Million) Advanced Computing and Communications Facility Operations Advanced Fusion Design Advanced Fusion Materials Research Alcator C-Mod Facility Operations Chemical Energy and Chemical Engineering Climate Change Technology Initiative (CCTI) DIII-D Facilities Operations Engineering Behavior Experimental Condensed Matter Physics Experimental Fusion Physics Support Experimental Plasma Research (Alternatives) Fusion Physics Research on Alcator C-Mod Fusion Physics Research on DIII-D Fusion Physics Research on NSTX Fusion Technologies Inertial Fusion Energy Research Mechanical Behavior and Radiation Effects NSTX Facility Operations Plasma Technologies Plasma Theory and Computation
Moderately Supportive RSPs (Combined Budget: $827.87 Million) Advanced Computing Software and Collaboratory Tools Atomic, Molecular, and Optical Science" Chemical Physics Research Cleanup Research Computer Science to Enable Scientific Computing Experimental Program to Stimulate Competitive Research (EPSCoR) General Plasma Science

General Purpose Plant & Equipment (GPP/GPE) High Performance Computer Networks Laboratory Technology Research and Advanced Energy Projects Mechanical Systems, Systems Science, and Engineering Analysis Multiprogram Energy Lab Facilities Support (MELFS) Neutron and Light Sources Facilities Physical Behavior of Materials Science Education Support Small Business Innovation Research (SBIR) Program Small Business Technology Transfer (STTR) Program Structure of Materials Theory & Simulations of Matter, Engineering Physics
NOTE: Please see Appendix A for more information on the budgets, the research performers, and other related information for each Research Summary.