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Collaborations Between BES and FE

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Abstract: This paper will show the organizational structure of the Department and the Office of Basic Energy Sciences. It will state the mission and fundamental tenets of this Office, its unique role within the context of U. S. government science funding, an overview of the program portfolio for the Metal, Ceramic and Engineering Sciences Team, and identify mechanisms for creating linkages outside of the Team, with particular emphasis on the distributed Center of Excellence for the Synthesis and Processing of Advanced Materials. Scientific achievements relevant to fossil energy materials needs that are discussed include the development of nickel and iron aluminide alloys, the interfacial adhesion of protective oxides grown on metallic substrates, the design and synthesis of ultrahigh-temperature silicides, and doubling the fracture toughness of silicon nitride.

Organizational Structure of the Department and the Office of Basic Energy Sciences

The Director of the DOE Office of Science is subject to nomination by the President and confirmation by the U. S. Senate. The present Director is Dr. Raymond L. Orbach. The Office of Science has a diverse portfolio in fundamental science including materials sciences, chemical sciences, biosciences, physics, life sciences, medical sciences, environmental sciences and mathematics and advanced computing. The Department is far and away the large source of federal support for user facilities for research and development, most of which are funded under the Office of Science.

One of the sub-offices under the Office of Science is the Office of Basic Energy Sciences. The Director for the Office of Basic Energy Sciences, Dr. Patricia M. Dehmer, is also an Associate Director for the Office of Science. The mission of the Office of Basic Energy Sciences may be divided into two categories:

- Foster and support fundamental research to provide the basis for new, improved, environmentally conscientious energy technologies.

- Plan, construct, and operate major scientific user facilities and serve user communities for researchers at universities, national laboratories and industrial laboratories.

The fundamental tenets of the Basic Energy Sciences program are:

Excellence in fundamental research

Relevance to the Nation's energy future, and

Stewardship to ensure stable, essential scientific communities, facilities, and institutions.

Excellent fundamental research produces new knowledge and ideas that

Change the way people think

Endure, and

Are widely used by others.

Basic Energy Sciences funds the larges collection of scientific user facilities for exploring the atomic world operated by a single organization. This collection includes four synchrotron radiation light sources, four high-flux neutron sources, four electron beam microcharaterization centers, a materials preparation center and a combustion research facility.

The President's budget that was requested for Basic Energy Sciences for Fiscal Year 2003 was $1,019.6 million. The major components of this request were as follows:

Construction of Facilities	$251.6 million
Operation of User Facilities	$244.6 million
Research at DOE Laboratories	$238.0 million
Research at Universities	$169.8 million

The activities under Basic Energy Sciences are divided into two divisions: Materials Sciences and Engineering Division and
Chemical Sciences, Geosciences and Biosciences Division. The activity under the Materials Sciences and Engineering Division is divided amongst two Teams. They are the Metal, Ceramic and Engineering Sciences Team and Condensed Matter Physics and Materials Chemistry Team.

Some web sites that provide further information are:

http://www.science.doe.gov/bes	(Office of Basic Energy Sciences)
http://www.science.doe.gov/bes/besstaff.html	(BES staff contacts and directory; click to organization chart)
http://www/science.doe.gov/bes/dms/dmshome.html	(Division of Materials Science and Engineering)
http://www.science.doe.gov/production/grants/grants.html	(Sponsored research details)
http://www/science.doe.gov	(Office of Science)

Program Portfolio under Metal, Ceramic and Engineering Sciences

Much of the program portfolio under Metal, Ceramic and Engineering Sciences underpins topics that are of critical importance to fossil energy systems. An overview of the Metal, Ceramic and Engineering Science portfolio shows that it may be represented by five core research activities as follows:

Structure and Composition of Materials

- Arrangement and identity of atoms and molecules in materials
- Development of quantitative characterization techniques
- Theory and modeling of atomic and magnetic structure
- Specialized tools for spatial resolution, quantitative imaging, and spectroscopy
- Mechanisms by which atomic arrangements are created and evolve
- Structure and composition of inhomogeneities including defects and the morphology of interfaces, surfaces and precipitates
- Advancing the state of the art of electron beam microcharacterization methods and instruments

Mechanical Behavior of Materials and Radiation Effects

- Behavior of materials under static and dynamic stresses
- Deformation and fracture over all length scales, temperatures and environments
- Relations among internal stress, crack nucleation, and crack tip shielding
- Response of materials to radiation resulting in atomic displacements
- Radiation damage mechanisms and degradation modeling
- Surface modification by ion implantation

Physical Behavior of Materials

- Response of materials to temperature, pressure, compositional gradients, and magnetic and electric fields
- Corrosion, electronic, magnetic, dielectric, semiconducting, and superconducting behaviors including role of defects and interfaces

Synthesis and Processing Science

- Atomic and molecular self-assembly
- Nanostructured materials that mimic the structure of natural materials
- Welding and joining
- New materials processing approaches to improve properties and reduce wastes

Engineering Sciences

- Materials engineering
- Nanotechnology and microelectromechanical systems (MEMS)
- Multiphase fluid dynamics and heat transfer
- Nonlinear, dynamic systems
- Non-destructive evaluation and early warning of impending failure

The Metal, Ceramic and Engineering Sciences portfolio is a significant and in some cases the only source of federal support for *fundamental scientific research* in the following energy mission relevant topics:

- Radiation damage
- Welding and joining
- Aqueous and galvanic corrosion
- High temperature gaseous corrosion
- Photovoltaic semiconductors
- High temperature mechanical behavior
- Non-destructive evaluation
- Granular and multiphase fluid transport
- Nonlinear behavior of engineering systems

There also are other activities under basic energy sciences that relate to fuel cells, catalysis and combustion.

Mechanisms for Linkages with Other Program Offices

The Metal, Ceramic and Engineering Sciences program has myriad linkages and interactions with other federal programs through distributed centers, formal coordinating committees, and participation in program reviews and joint workshops. A few examples are:

- Center of Excellence for the Synthesis and Processing of Advanced Materials
- Computational Materials Sciences Network
- Nanotechnology Network (with National Nuclear Security Agency)
- Energy Materials Coordinating Committee
- MatTec Working Group on Structural Ceramics
- MatTec Working Group on Metals
- MatTec Working Group on Nondestructive Evaluation
- Participation in program reviews for DOE technology programs such as Photovoltaics, Superconductivity, and Industrial Materials
- Join workshops

The Center of Excellence for the Synthesis and Processing of Advanced Materials

This distributed Center referred to as the CSP is a coordinated and cooperative venture among 12 DOE Laboratories, and university and industrial partners. It was established in response to the recognition of the enabling role of materials synthesis and processing in fulfilling the Department's mission needs. The latter call for advanced materials that can reliably satisfy performance requirements for various energy generation, conversion and conservation technologies. The objective of the CSP is to enhance the science and engineering of materials synthesis and processing in order to meet programmatic needs of the Department and to facilitate the technological exploitation of materials. The CSP capitalizes on the complementary strengths of the participating institutions to solve important problems. It has a technology perspective, which is provided by a Technology Steering Group.

There are five selection criteria that must all be satisfied for a project to qualify for participation under the CSP:

- Scientific excellence
- Clear relationship to energy-related technologies
- Involvement of several laboratories
- Existing or potential partnerships with DOE Technologies-funded programs, and
- Existing or potential in-kind partnerships with industry

The criterion by which the performance of the CSP is evaluated is the amount by which the total integrated output of a CSP project exceeds the sum of the isolated non-interactive components of the project.

The CSP presently funds the following eight projects:

- High Efficiency Photovoltaics
- Design and Synthesis of Ultrahigh-Temperature Intermetallics
- Isolated and Collective Phenomena in Nanocomposite Magnets
- Controlled Defect Structures in Rare-Earth Ba-Cu-O Cuprate Superconductors
- Interfacial Adhesion Related to Protective Oxides Grown on Metallic Substrates
- The Science of Localized Corrosion
- Smart Structures Based on Electroactive Polymers
- Nanoscale Phenomena in Perovskite Thin Films

Intermetallic Nickel-Aluminide and Iron-Aluminide Alloys: An Integrated Materials Research Success Story

An example of successful integration of materials research at Oak Ridge National Laboratory is intermetallic alloys. Basic and applied materials research programs, together with industrial collaborations, played essential roles in the successful development of nickel- and iron- aluminides for industrial applications. Beginning in 1981, exploratory (Laboratory-Directed Research and Development) and Basic Energy Sciences funds were used to discover a method to ductilize nickel aluminide by the addition of boron, to determine the optimum nickel to aluminum ratio, and to understand the fundamentals of intergranular embrittlement in these alloys so as to develop a scientific basis for improving their properties. Within two years, applied research programs initiated complementary projects to develop commercial alloys for industrial uses. For example, research funded by the Assistant Secretary for Energy Efficiency and Renewable Energy expanded the fundamental research efforts by sponsoring the development of nickel-aluminide alloys with high-temperature strength and corrosion resistance. These efforts resulted in the first commercial license in 1985 to Cummins Engine Company, Inc., for the production of nickel-aluminide, precision-cast turbocharger rotors. Similarly, the Assistant Secretary for Fossil Energy supported the development of iron-modified nickel aluminides for applications in coal conversion (sulfidizing) environments.

As these programs grew, industry identified new applications and challenges for an improved fundamental understanding of the aluminides. Beginning in 1989, partnerships with industry, based on both applied and fundamental research, were accelerated by the introduction of Cooperative Research and Development Agreements (CRADAs). The number and quality of scientific publications and the number of industrial agreements can measure the success of the integrated aluminide materials research program, which exemplifies one of the strengths of the Department of Energy National Laboratory system. More than 50 refereed publications per year, over 350 citations to aluminide research per year, and the introduction of a new scientific journal (*Intermetallics*) demonstrate the importance and the breadth of the intermetallic alloy scientific program. The technological significance is exemplified by the 13 licenses and 7 CRADAs that have evolved from the efforts to develop an understanding of embrittlement in aluminides. Commercial products include dies for the manufacture of "super" magnets (produced by Metallamics, in use at General Motors' (GM) Magnequench facility and others), rolls for annealing furnaces (under evaluation at a major steel company, part of a CRADA with Metallamics), and furnace trays (under evaluation at GM). In all of these applications, use of the intermetallic alloy has extended the lifetime and improved the performance of the component.

CSP Project Interfacial Adhesion Related to Protective Oxides Grown on Metallic Substrates

The CSP project *Interfacial Adhesion Related to Protective Oxides Grown on Metallic Substrates* has the objective of furthering the fundamental understanding of the interfacial bonding and dynamics that underlie oxide-metal adhesion and the energetics associated with decohesion for systems relying on protective alumina coatings. This project employs theoretical calculations, experiments and modeling. Three recent highlights from it are as follows:

Micro x-ray photoelectron spectroscopy studies have identified the segregants and their chemical state at the alloy/Al_2O_3 interface for two different iron-based high temperature alloys. While both alloys form the same oxide film, the nature of the interfacial segregants are substantially different.

Synchrotron x-ray measurements were used for rapid determination of strain in thin chromia films formed by the high temperature oxidation of an Fe-Ni-Cr alloy. Large strains can lead to decohesion at the metal/oxide interface.

Finite element continuum models were developed to analyze surface and interface cracking of protective oxides at regions of local curvature (e.g., corners) during cooling from high temperature. The results have lead to an improved understanding of failure mechanisms and local fracture behavior.

CSP Project Design and Synthesis of Ultrahigh-Temperature (Silicide) Intermetallics

The CSP project *Design and Synthesis of Ultrahigh-Temperature (Silicide) Intermetallics* seeks to generate the knowledge required to establish a scientific basis for the design and processing of transition-metal silicides and materials based on silicides for structural applications at temperatures of 1400^0C and above.

The substitution of Nb or V for Mo in Mo_5Si_3 greatly reduces the coefficient of thermal expansion (CTE) anisotropy between the *c*- and *a*-axes of Mo_5Si_3 in agreement with *ab initio* theoretical calculations. The CTE ratio, CTE(c)/CTE(a) is reduced from 2 for Mo_5Si_3 to 1.5 for both Mo_4NbSi_3 and Mo_4VSi_3.

It has been shown that the boron-modified molybdenum silicide alloy, Mo-12Si-8.5B (at.%), can be processed to be considerable tougher and more fatigue resistant than both monolithic $MoSi_2$ and Nb-sphere reinforced $MoSi_2$. Additionally, the crack-growth resistance of this B-modified alloy increases progressively with increasing temperature up to 1300^0C.

A process to improve the fracture toughness of Mo-Si-B alloys has been developed and demonstrated for a Mo-20Si-10B (at.%) alloy. The process is based on the consolidation of Mo-coated Mo-Si-B particles leading to the formation of Mo_3Si and Mo_5SiB_2 phases in a continuous alpha-Mo matrix.

Precise Location of Additive Atoms Shown to Double Fracture Toughness of Silicon Nitride Ceramic

Unprecedented high-resolution transmission electron microscopy studies using new image acquisition and analysis techniques that yield sub-Angstrom resolution have linked the mechanical properties of a silicon nitride ceramic to the exact location of additive atoms in the grain boundaries. The result was obtained for Si_3N_4 containing a precisely controlled sintering additive, 2 wt.% yttrium oxide. Heat treatment led to a ~ 100% increase in fracture toughness (the ability to resist brittle fracture) and a change in the fracture mechanism. The elevation in toughness results from weakening of the grain boundaries, caused by the segregation of yttrium there. This causes fracture to occur along the grain boundaries, which toughens the material. Direct visualization of atoms in the crystal structure and especially along the boundaries confirmed the theoretically predicted location of segregated yttrium atoms at the intergranular interface. This result is very significant for the understanding of interfacial bonding and therefore mechanical properties. Direct visualization of the yttrium atoms has shown that minute changes in atom location have a large effect on the strength of grain boundaries and therefore a profound influence on the fracture toughness of ceramics. R. Ritchie and C. Kisielowski at the Lawrence Berkeley National Laboratory performed this research.