AIR FORCE OFFICE of SCIENTIFIC RESEARCH [AFOSR]
Manager of the Basic Research Investment for the Air Force

Research HIGHLIGHTS

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AFOSR Success Story

The Air Force Perchlorate Model

An Air Force Office of Scientific Research funded initiative results in a successful system for the treatment of the hazardous environmental contaminant known as ammonium perchlorate.

Ammonium perchlorate serves as an essential component of solid rocket fuel and plays an important role in the performance of the U.S. Intercontinental Ballistic Missile (ICBM) Fleet. However, this oxidant exists as an environmental contaminant requiring stringent control.

In the late 1980s, the environmental concerns relating to ammonium perchlorate were made particularly acute. Many pressures were placed on the U.S. Air Force through international treaties and emerging environmental requirements to treat wastes related to propellant disposal.

At that time, Air Force scientists, at the Air Force Engineering and Services Center at Tyndall AFB in Florida, recognized environmental concerns related to ammonium perchlorate. The disposal and refurbishment requirements of the ICBM fleet needed new procedures to convert the ammonium perchlorate to innocuous products. Dr. Jim Cornette, Capt. Mark Smith, and Dr. Hubert Attaway began work on this problem. They searched for a way to convert this strong oxidizer into a harmless substance as quickly and simply as possible.

The quest was significantly aided by the team's 1989 discovery of a microorganism that apparently converted the perchlorate ion to a chloride, or simple salt. This unique conversion occurs at room temperature, under extremely mild conditions, thus preventing production of hazardous materials that often occurs with other procedures.

This led AFOSR to fund further investigation of the observation from 1989 to 1991. AFOSR's support helped confirm the team's initial findings, and led to a scaled-up version of the process. The development ensured the conversion was possible when scaled up.

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Pilot-scale Perchlorate Bioreactor System installed and operated at Tyndall AFB, Florida

Atomic Structure Models Provide Link to Predictions of Properties of Materials

The Air Force Office of Scientific Research (AFOSR) sponsored research resulting in a dramatic verification of the accuracy of a model that provides the capability to predict certain aspects of the deformation behavior of metals. This discovery will allow the Air Force to vastly decrease the scope, duration and thus, cost, of testing materials used in weapon systems.

BACKGROUND INFORMATION

Many useful engineering properties of materials depend on the type and distribution of defects in the arrangements of their atoms. While experiments are required to establish and validate materials, databases used in design and selective use of computations using physically based models can vastly decrease the scope, duration and cost of experimental programs. This computational strategy provides the foundation for programs leading to shorter design cycles that incorporate optimized techniques for materials selection and processing, resulting in more affordable and reliable weapons systems.

Dislocations are the principal crystal defect responsible for permanent changes in shape of crystalline materials. Atomic models of dislocations based on quantum mechanics provide the information necessary to explain and predict differences in the deformation behavior of various metals. This information forms the basis for computational models that relate the behavior of a material to its thermo-mechanical environment, permitting computations of structure and property changes during processing and service. Experimental verification of structures based on models increases confidence in the prediction of other properties that are more difficult to measure.

AFOSR-SPONSORED MODELLING AND EXPERIMENTAL VERIFICATION

Since 1998, the Metallic Materials program in the Aerospace and Materials Sciences Directorate of the Air Force Office of Scientific Research (AFOSR/NA), have funded two universities involved in the determination of atomic core structure of dislocations in various metals.

First, Professor Arthur Freeman and his colleagues at Northwestern University, created a first-principles model that forecasts the atomic core structure of dislocations in gold and iridium.

Then, using High Resolution Transmission Electron Microscopy (HRTEM), Professor Kevin Hemker and associates at Johns Hopkins University achieved direct resolution of dislocation cores in gold and iridium. The results of Hemker's team proved that previous calculations by Freeman's group accurately forecasted atomic positions around dislocation cores for several different dislocation configurations.

Figure 1 compares actual and calculated locations of atoms around dislocations in gold and iridium. In all cases the bright spots correspond to the intersection of parallel columns of atoms with the plane of the picture. Arrows on the atoms show the relative magnitude and displacements of the atoms from their positions in a perfect crystal. The similarity of the array of arrows for the experimental and calculated images illustrates the excellent agreement between theory and experiment. Differences in the array of arrows in the two metals are due to differences in the atomic bonding characteristics of the materials.

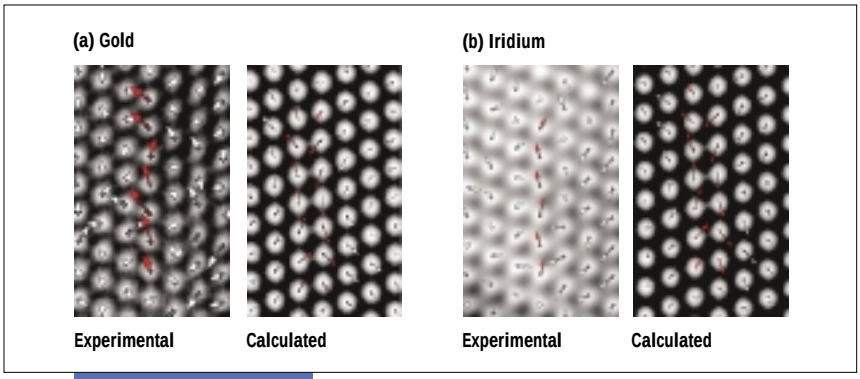

FIGURE 1:
Images of Screw Dislocation Cores in Gold and Iridium

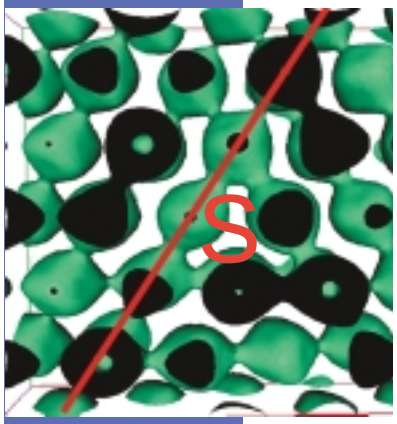

FIGURE 2:
Iso-charge density plot showing atomic locations around the core of a screw dislocation in Molybdenum

This extramural research is complemented by an intramural program at the Air Force Research Laboratory's Materials and Manufacturing Directorate under the leadership of Dr. Dennis Dimiduk. In this program, researchers have developed a hybrid model that couples discrete and continuum descriptions of the crystal to calculate dislocation core structures in molybdenum (Mo).

Figure 2 shows the results of their calculations for the atomic arrangement around a screw dislocation in molybdenum.

Presently, research is being conducted in Hemker's laboratory at Johns Hopkins to verify this structure in a manner similar to the experiments on gold and iridium.

Results of this research will extend the capability for linking deformation behavior of these metals to their atomic structure, thus expanding our capability for constructing accurate models for the design of materials, thereby reducing costs of new materials.

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The Engineer and Scientist Exchange Program

PART 1

For many years, the Air Force Office of Scientific Research (AFOSR) has played a critical implementation role in the Air Force's Engineer and Scientist Exchange Program. (ESEP)

The ESEP program is a Department of Defense (DoD) initiative promoting international cooperation in military research, development and acquisition of technology. The Air Force centrally maintains the only managed ESEP program. The Deputy Under Secretary of the Air Force, International Affairs (SAF/IA) provides policy guidance for the program. The Air Force Office of Scientific Research's External Programs and Resources Interface Directorate (AFOSR/NI) manages the placement of all ESEP participants and implements all support actions for USAF participants. AFOSR field offices in London and Tokyo act as overseas program liaison centers for ESEP personnel working in Europe and Asia respectively.

Since 1963, AFOSR has coordinated on-site working assignments for US military and civilian engineers and scientists in allied and friendly government organizations and the reciprocal assignment of foreign engineers and scientists in US defense establishments. This program provides invaluable experience gained in international research, development and acquisition along with important personal connections with people and research institutions.

In most cases, participants work hands-on research projects rather than simply observing others do the work. In fact, participants are expected to become an integral part of the host organization's work. ESEP participants both contribute to and learn from host country scientists and engineers as they work together in defense efforts of mutual interest to both nations.

Air Force personnel compete in a highly selective process. Every two years approximately eight individuals are selected for this unique opportunity. Assignments are normally for two years, and may be preceded by six months of language training.

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Current ESEP Participants:

FRONT, L to R: Dr. Joseph C. Sturgis, Capt. Brian Quillen, Capt. Richard Branam

BACK, L to R: Capt. Richard Salasovich, Maj. Matthew Bohn, Capt. Derek Ebdon, Capt. Matthew Yocum

AFOSR Success Story

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The investigation's success prompted the Air Force to provide advanced developmental funding support for the program. The result—a clear demonstration of the potential for this innovative process.

In 1993, this innovation caught the attention of the Joint Ordnance Commander's Group (JOCG), a joint service group charged with disposal of ammunition stockpiles. The JOCG supplemented Air Force funding and permitted further scale-up of the process resulting in the construction and demonstration of a prototype biological reactor system.

During 1995, the reactor system was further refined at the Tyndall AFB, Air Force Research Laboratory, Materials and Manufacturing Directorate (AFRL/MLQ), and then installed at the Thiokol rocket production facility in Bringham City, Utah. This installation allowed the facility to meet regulatory requirements for contaminated water effluent processing related to the regraining of fuels for the Minuteman ICBM fleet. In addition, the treatment process supported perchlorate recovery and reuse, which further reduced the Minuteman system regraining cost. The treatment system successfully operated at the Thiokol facility for almost three years without failure.

As a final result, an Air Force patent for this process has been licensed to industry. One of the major suppliers to the military of ammonium perchlorate has reached an agreement with the Air Force licensed contractor. The agreement allows the decontamination of sites that threaten water supplies.

As the contractor improves the perchlorate treatment process and incorporates improvements into the system, the Air Force license agreement provides royalty free use of the new innovations. In this way, we reduce the operational cost of the system by ninety percent.

This innovative program has been widely cited within the Air Force environmental community and sister services as the "Air Force Perchlorate Model." This model progressed from initial discovery of the microorganism to practical implementation of the technology in a period of seven years.

"It clearly shows the essential role that AFOSR, other funding agencies, and industry play in ensuring the most efficient process comes to fruition," commented Dr. Jim Cornette, Deputy Chief, Air Expeditionary Forces Technologies Division, AFRL/MLQ, on this successful program.

For his efforts in managing this technology development program and successful transition, Mr. James Hurley, AFRL/MLQ, received the Lt. General Thomas M. Ferguson Award for Technology Transition. The Air Force Materiel Command (AFMC) gives this award annually to the AFMC engineer or scientist who demonstrates the most innovative and significant technology transfer in the entire Command.

The Engineer and Scientist Exchange Program

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PART 2

Some Highlights for five of AFOSR's current ESEP participants.

Capt. Brian Quillen, Chief, Gas/Chemical Laser Branch, AFRL/DE, Kirtland AFB, NM, directed operations of DoD's lead laboratory for high power laser weapons/applications. Under the Engineer and Scientist Exchange Program, he is assigned to the Technical Physics Institute at Deutsches Zentrum fur Luft und Raumfahrt (DLR) in Stuggart, Germany. He conducts research on the technology advancement for the Chemical Oxygen-Iodine Laser (COIL).

Capt Matthew Bohn, Assistant Professor of Mathematical Sciences, U.S. Air Force Academy, CO, was also a principle investigator for an AFOSR research project. Currently he conducts laser ESEP research at DLR in Stuggart, Germany.

Capt. Derek Ebdon, a USAF Lead Aircraft Battle Damage Repair (ABDR) Engineer and ABDR Program Manager, managed all ABDR technology efforts and engineering requirements for the U.S. Air Force. Currently, through ESEP he is assigned to DCSD, ONERA in Toulouse, France where he evaluates the active use of flexibility for new aircraft concepts.

Larry Lewis, a Chief for the AFRL/MN Flyout Team, directed a team to provide effective munition and analysis to support Directorate R&D technology programs. Currently, through ESEP he is assigned to the Department of Defense and Science Technology Organization in Australia. Specifically, he works with the Weapons Systems Division and Weapons Systems Analysis group at the Aeronautical and Maritime Research Laboratory.

Capt. Richard Salasovich, a Squadron Section Commander at AFRL/PR, Edwards AFB, CA, oversees Edwards Research Site military manpower, performance, and award actions for a 70-member military unit. Currently, through ESEP, he is assigned to Deutsches Zentrum fur Luft und Raumfahrt e.v. (DLR) where he conducts aerospace research.

For more information on the ESEP Program, please contact the External Programs and Resources Interface Directorate at 703-696-7300 and request an ESEP brochure. In the near future, you may obtain further information at AFOSR's website at **afosr.sciencewise.com.**

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AFOSR would like to thank Dr. Jim Cornette, Dr. Craig Hartley, Mr. Joe Niksic, and Ms. Nahaku McFadden for their assistance in making this issue possible.

Research Highlights is published every two months by the Air Force Office of Scientific Research. This newsletter provides brief descriptions of AFOSR basic research activities including topics such as research accomplishments, examples of technology transitions and technology transfer, notable peer recognition awards and honors, and other research program achievements. The purpose is to provide Air Force, DoD, government, industry and university communities with brief accounts to illustrate AFOSR support of the Air Force mission. *Research Highlights* is available on-line at:

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