

2005

University of Nevada, Las Vegas Transmutation Research Program: Annual Report Academic Year 2004-2005

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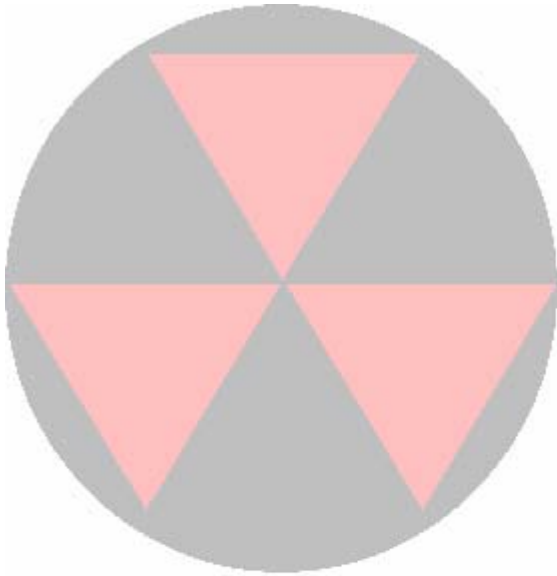
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University of Nevada, Las Vegas
Transmutation Research Program
Annual Report
Academic Year 2004-2005

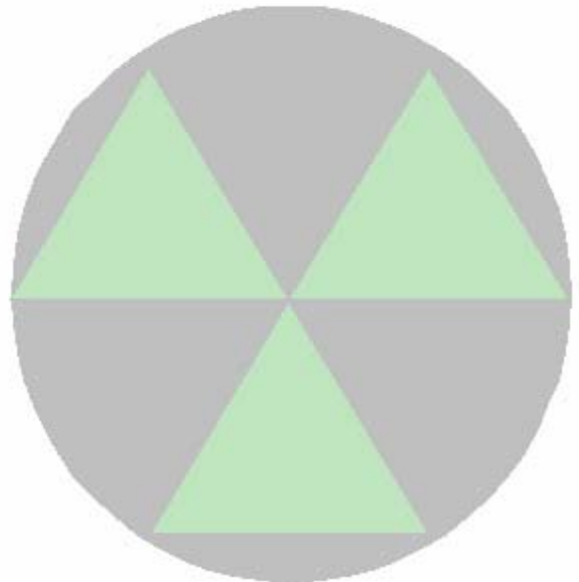


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Letter from the Director



Anthony E. Hechanova, Ph.D.
Director, UNLV Transmutation Research Program



It is my pleasure to present the UNLV Transmutation Research Program's fourth annual report that highlights the academic year 2004 – 2005. Supporting this document are the many technical reports and scientific papers that have been generated over the past three years, which can be found on our program's website at <http://aaa.nevada.edu>.

In the fourth year of our program, we added 11 new research tasks and saw the conclusion of 8 of the initial 16 independent student research tasks started in 2001 and 2002. In all, the program has sponsored to their conclusion 28 M.S. and 2 Ph.D. degrees. The program supported 58 graduate students and 13 undergraduates in 6 academic departments across the UNLV scientific and engineering communities in the academic year 2004-2005.

Our research tasks span the range of technology areas for transmutation, including separation of actinides from spent nuclear fuel, methods of fuel fabrication, reactor-accelerator coupled experiments, and corrosion of materials exposed to lead-bismuth eutectic.

In order to continue the growth and vitality of the research effort at UNLV, we also invested in our academic and research infrastructure. We saw the initiation of two new academic programs Fall term 2004: a Ph.D. program in Radiochemistry and an M.S. program in Materials and Nuclear Engineering. We continued our emphasis on molten metal technology and actinide chemistry in our enhancements to UNLV this year to build a foundation in areas that are in line with UNLV's strategic growth and our ability to address student-appropriate research in the transmutation program.

Finally, I believe that through the Transmutation Research Program, UNLV has established itself as the core university participant in transmutation research with active collaboration with national laboratories, universities, and international institutions.

I congratulate our students and faculty on a job well done and I look forward to the opportunities and challenges of this exciting research endeavor.

Sincerely,

A handwritten signature in black ink that reads "Anthony E. Hechanova". The signature is written in a cursive style and is positioned to the left of a vertical red line.



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UNLV Transmutation Research

The UNLV Transmutation Research Program was established in March 2001 as part of the national transmutation program (currently called the Advanced Fuel Cycle Initiative of the U.S. Department of Energy, Office of Nuclear Energy, Science and Technology) to develop the technologies necessary for the ecological and economical treatment of spent nuclear fuel.

The goal of the UNLV program is to develop a sustainable and robust research community at UNLV that is able to contribute to and support the national effort through faculty-supervised, student-conducted research. In establishing the UNLV program, four basic principles were followed: peer review, program focus, integration with the national program, and commitment to the long-term goals of transmutation.

The primary role of the UNLV program in the national effort is the training of graduate and undergraduate students in nuclear engineering and other related fields to support the augmentation of the human infrastructure for transmutation technologies. However, the research conducted by UNLV faculty and students is also an integral part of the national research effort. This is accomplished through the direct involvement of students in collaborative research supporting the national transmutation research and development program.



UNLV students discuss their research with international scientists at the Eighth Annual OECD/NEA Actinide and Fission Product Partitioning and Transmutation meeting held at UNLV November 9-11, 2004.

Twenty-seven independent student research tasks, supporting 58 graduate students and 13 undergraduates, were ongoing or concluding this academic year. The UNLV program includes the involvement of 32 faculty in 6 academic departments.

UNLV research tasks span the range of technology areas for transmutation: separations of used fuel materials, fuel fabrication, accelerator design, materials corrosion and performance, neutron multiplicity and transport simulations and experiments, and research in lead-bismuth eutectic technology development.



Undergraduate student Amber Wright with a new Inductively Coupled Plasma Atomic Emissions Spectrometer (ICP-AES) installed on November 16, 2004. Wright will be entering the Radiochemistry Ph.D. program Fall 2005 and was one of eight students nationwide to receive an AFCI fellowship.



20 UNLV students toured the Palo Verde Nuclear Generating Station in Wintersburg, AZ, the largest nuclear electric generating site in the U.S. on March 25, 2005.

Program Overview

The UNLV Transmutation Research Program consists of four components: Program Support, Research Infrastructure Augmentation, International Collaboration, and Student Research.

In the first year of the program, the student research component was supported by the infrastructure augmentation and the program support components. In the second year of the program, the fourth leg of the support system, international collaborations, was added to the research support system.

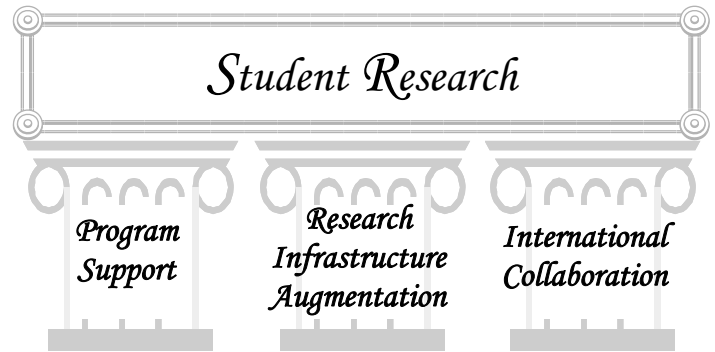
These components are responsible for all aspects of the program that are not directly related to the student research projects, such as hiring new faculty, bringing new research equipment to campus, assisting the development of new student research projects, coordinating with the national program, coordinating with the international research programs, as well as the typical administrative details of a program of this size.

The primary goals of these components are to support the current UNLV research efforts in transmutation technologies, to augment faculty and staff, and to increase research infrastructure necessary for the strategic growth of the UNLV research mission.

Through the infrastructure augmentation component, this year, the UNLV program completed a new Actinide Chemistry Laboratory and an Inductively Coupled Plasma – Atomic Emission Spectroscopy User Facility. The program also continued the development of facilities for working with molten lead-bismuth (a nuclear coolant and target material).

Two new academic programs started Fall term 2004: a Ph.D. in Radiochemistry and an M.S. in Materials and Nuclear Engineering, the latter mentioned in Sen. Pete Domenici's recent book.

The infrastructure augmentation component also supported the addition of new research faculty: Prof. Jian Ma who coordinates the TRP lead-bismuth loop projects and Prof. Thomas Hartmann who leads the HRC Structure and Solid Phase Analytical Group. The program also continues to support the Nevada Center for Advanced Computational Methods faculty Prof. Yitung Chen in addition to other faculty members highlighted in past reports.

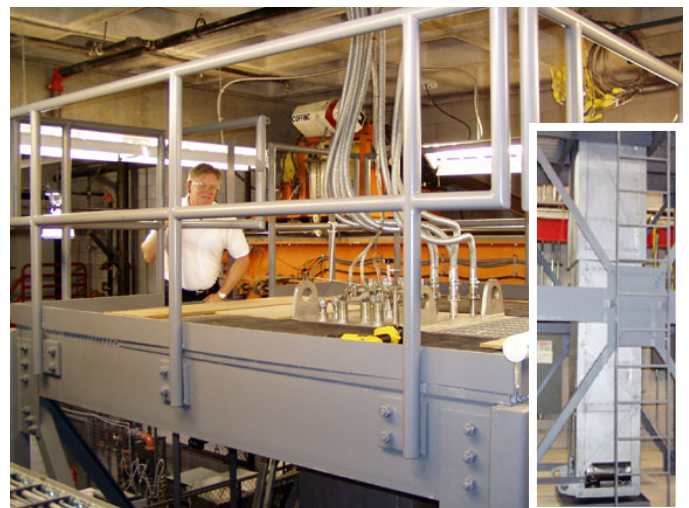


UNLV Transmutation Research Program Components

Through the international collaborations component, the program hosted a team of Russian scientists from the Institute for Physics and Power Engineering in Obninsk, Russia, who came to continue the installation of the Russian-built lead-bismuth loop.

The international collaboration component also supported three joint research proposals: two between UNLV and the Khlopin Radium Institute (UNLV Tasks 15 and 16) and one with the Ben Gurion University of the Negev (Task 19).

The program support component sponsored a number of workshops and meetings this year between UNLV researchers and scientists from our national laboratory partners and the international community (in particular, the OECD/NEA Partitioning and Transmutation conference) for the development of transmutation technologies, as well as sponsoring the participation of 13 UNLV students in the ANS Student Conference at Columbus, Ohio.



International Programs Adviser Thomas Ward views the electrical connections atop the Russian-built molten metal loop (inset) in the UNLV Howard Hughes College of Engineering.

Transmutation at a Glance

Introduction

Over 20% of the electricity generated in the U.S. is provided by nuclear power reactors. It is estimated that the amount of used nuclear fuel in the U.S. will reach 140,000 tons by the end of the operational period of current reactors.

Many countries take different approaches to the management and recycling of used nuclear reactor fuel. The U.S. is pursuing a strategy of waste management that would place used nuclear fuel in deep geologic repositories for a long time, separating it from the biosphere and allowing the radioactive isotopes of the waste to decay to more stable progeny.

Transmutation is an alternative waste management strategy undergoing research and development in the U.S. The new national program was authorized by Congress to begin in fiscal year 2001, as the Advanced Accelerator Applications program. In fiscal year 2002, the national program was continued and expanded by Congress, and renamed the Advanced Fuel Cycle Initiative (AFCI) program. The goals of the national program are to develop fuel cycle technologies that:

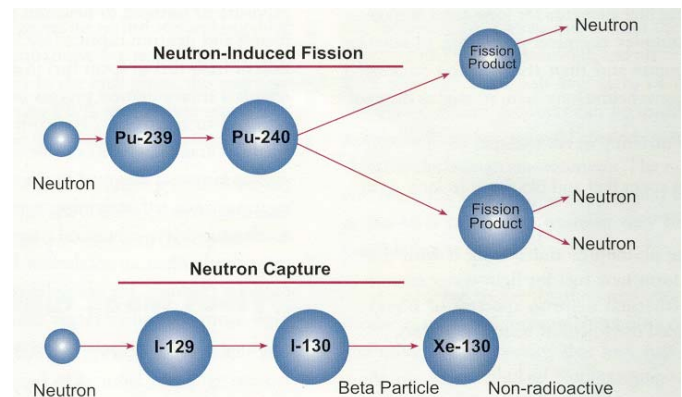
- Enable recovery of the energy value from commercial used nuclear fuel,
- Reduce the toxicity of high-level radioactive waste bound for geologic disposal,
- Reduce the inventories of civilian plutonium in the U.S., and
- Enable more effective use of the currently proposed geologic repository and reduce the cost of geologic disposal.

The transmutation concept could provide a dramatic shift in the U.S. waste management strategy by lessening the inventory of residual radioactivity, allowing recycling of fuel, providing optimization of final waste forms, and potentially removing much of the material from Nevada.

What is Nuclear Transmutation?

For centuries, alchemists have been trying to transform elements into other elements, primarily lead into gold. With modern nuclear science, we can finally accomplish this. Scientists are using nuclear transmutation to change one isotope into another more favorable isotope by changing its nuclear structure. This process for waste management is aimed at plutonium, other actinides, and long-lived fission products, with the ultimate goal of converting them into short-lived isotopes that can be managed over a reasonable timeframe.

Transmutation can be done with two different processes: neutron-induced fission and neutron capture. Both processes start with the target nucleus absorbing an incident neutron. After the neutron is absorbed by the target nucleus, the nucleus can either fission (splitting of the nucleus) or go through another nuclear transmutation process such as radioactive decay. Both processes lead to the same final result: transmutation of waste. These processes are illustrated in the figure below.

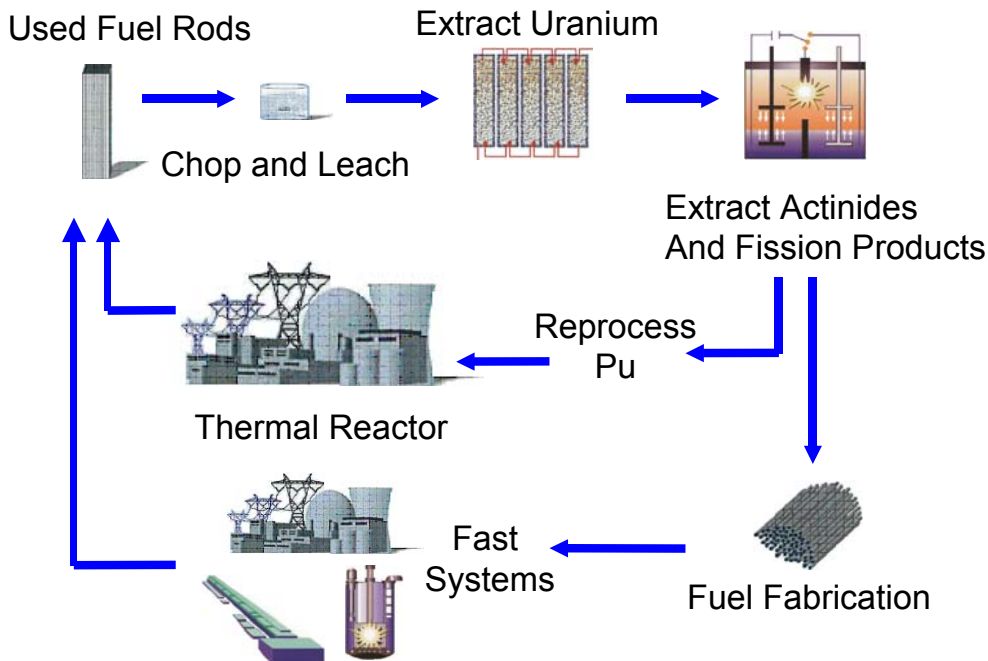


This picture illustrates how neutrons are used to transmute actinides and fission products.

Neutron-Induced Fission (top): a neutron is captured by a fissile actinide (e.g. Plutonium-239) and is induced to split (or fission).

Neutron Capture (bottom): a neutron is captured by a nucleus (e.g. Iodine-129). A new nucleus is produced, Iodine-130, which decays into Xenon-130 which is a stable isotope (i.e., not radioactive). This decay process is complete within a few days.

Multi-tier Transmutation Concept



The above figure shows how used nuclear fuel could be managed under a multi-tiered transmutation strategy. In the first tier, plutonium (and other fissile actinides) would be recycled from used fuel and transmuted in a new advanced thermal reactor. In the second tier, remaining long-lived radioactive isotopes would be transmuted using a fast spectrum reactor and/or accelerator-driven system.

REDUCE, REUSE, RECYCLE, RESEARCH

Benefits from Transmuting Nuclear Waste

Many benefits are obtained from transmutation of nuclear waste. Some of them are:

(1) The initial amount of high-level radioactive waste will be reduced by virtue of separation (only two percent of used nuclear fuel is highly radioactive, the rest, if separated, can be classified as low-level or non-radioactive).

(2) The radiotoxicity of the residual waste will be reduced such that it could be less radiotoxic after 300 years than direct disposal of used nuclear fuel after 100,000 years.

(3) Usable energy is produced by destroying hazardous components of used nuclear fuel. Plutonium and other isotopes can be continuously recycled.

(4) Someday other used nuclear fuel materials, such as uranium, may be reused. It is possible that other isotopes separated from nuclear waste could have a useful purpose in medicine and industry.

(5) The accelerator process will provide a powerful proton source that could be used in medical therapy and to produce isotopes for a variety of applications such as: medical isotopes, industrial isotopes and research isotopes.

Task 1

Design and Analysis of a Process for Melt Casting Metallic Fuel Pins Incorporating Volatile Actinides

Y. Chen, D.W. Pepper, and R. Clarksean

BACKGROUND

The incorporation of non-fertile actinides into a fuel matrix for a transmuter blanket is of interest to the Advanced Fuel Cycle Initiative. One of three proposed candidate matrices for the transmuter is a metallic alloy fuel matrix. Metallic fuels are an outstanding candidate for a transmutation fuel due to excellent irradiation performance and ease of fabrication. However, incorporating a volatile constituent during fabrication of these or other fuel pins presents a challenge.

Volatile actinides, particularly americium, are susceptible to rapid vaporization during the traditional metal fuel casting processes. The actinide vapors boil off, and flow out of the system into the off-gas recovery system, resulting in only a fraction of the volatile actinide charge being incorporated into the fuel pins. The loss of these actinides from the fuel greatly complicates the task of preparing them for transmutation, requiring additional recovery and fuel fabrication steps to try to incorporate the volatile actinides into the transmuter fuel.

RESEARCH OBJECTIVES AND METHODS

The goal of this project is to investigate the casting processes for metallic fuels to help design a process that minimizes the loss of the volatile actinide elements from the fuel. The research effort centers on the development of advanced numerical models to assess conditions that significantly impact the transport of volatile actinides during the melt casting process and represents a joint effort between researchers at UNLV and Argonne National Laboratory (ANL). Assessing critical equipment and process variables is required to build a successful system that will operate efficiently.

RESEARCH ACCOMPLISHMENTS

Development of the induction-heating model: Modeling efforts centered on the development of the governing equations, incorporating these equations into computer codes, setting up a test problem, and making preliminary calculations for the geometry of interest. Detailed analyses were conducted for an Induction Skull Melter (ISM) previously built and tested by ANL.

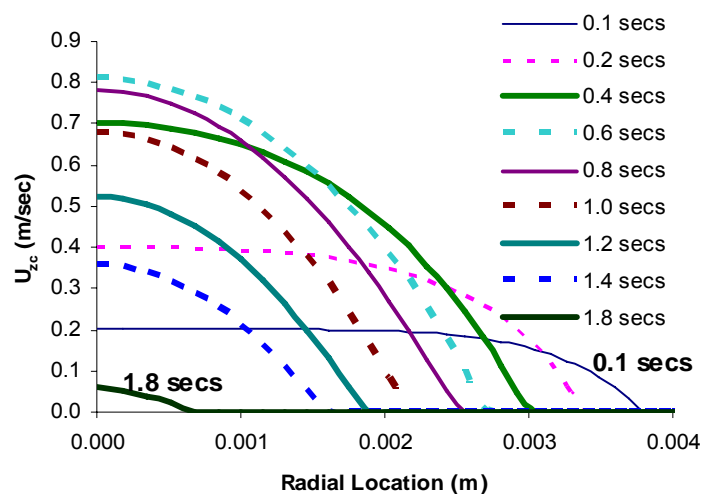
Modeling of casting process: Efforts continued to improve a model for the casting of fuel pins. Work considered the flow of the melt into the mold and heat transfer into the mold during solidification (after flow has stopped). Results from an energy balance model indicate that the thermal mass would typically be greater than needed to solidify the melt within the mold. The results of this simple model have aided in designing a

mold to hold and solidify the fuel pins. Detailed flow and heat transfer models show how the melt flows into the mold and ultimately solidifies.

In order to test the impact of process parameters (temperature, pressure, alloying elements, etc.) on the casting process, parametric studies were carried on different processing parameters. These studies centered around model development and analysis of the impact of mold preheating on heat transfer into the model. Results will assist with determining which process parameters are critical in manufacturing a suitable metallic fuel pin.

Americium Transport Models: A model that analyzes the transport of americium from the melt to the vapor phases above the crucible has also been developed. The model considers mass transport in the melt, vaporization at the surface, and transport through the vapor phase. Parametric studies are underway to evaluate the impact of different properties or situations on the transport of americium from the melt.

Develop Prototype Furnace Design: A preliminary furnace design that can be built and tested with surrogate materials is critical in order to assess the viability of metal fuels. A preliminary analysis of potential surrogate materials has been completed. Manganese appears to be an acceptable surrogate material. Discussions will be held with Argonne National Laboratory staff members to insure that no health and safety issues prevent manganese from being used in future tests.



Axial velocity profile for constant inlet pressure of 20 kPa
(Mold temperature = 400°C, initial melt temperature = 1500 °C, interfacial heat transfer coefficient = 2,000 W/m²-K).

TASK 1 PROFILE

Start Date: June 2001

Completion Date: June 2004

Theses Generated:

Xiaolong Wu, M.S., Mechanical Engineering, "Design and Analysis for Melt Casting Metallic Fuel Pins Incorporating Volatile Actinides," August 2002.

Taide Tan, M.S., Mechanical Engineering, "Design and Simulation of an Induction Skull Melting System," May 2004.

Journal Article:

T. Tan, R. Clarksean, Y. Chen, S. Hsieh, and M. Meyer, 2004, "Simulation of the Casting Process for Melt Casting a Metallic Fuel Pin," submitted to *Nuclear Engineering and Design* – under review.

Conference Proceedings:

T. Tan, R. Clarksean, Y. Chen, S. Hsieh, and M. Meyer, "Analyzing a Process for Casting Volatile Actinides," *6th International Topical Meeting on Nuclear Reactor Thermal Hydraulics, Operations and Safety*, Nara, Japan, October 4-8, 2004.

T. Tan, R. Clarksean, Y. Chen, S. Hsieh, S., and M. Meyer, "Numerical Simulation of an Induction Heating Process in an Induction Skull Melting Furnace," *ICHMT International Symposium on Advances in Computational Heat Transfer*, Norway, April 19-24, 2004.

T. Tan, R. Clarksean, Y. Chen, S. Hsieh, and M. Meyer, "Simulating the Casting Process for Melt Casting a Metallic Fuel Pin," *12th International Conference on Nuclear Engineering (ICONE-12)*, Arlington, VA, 25-29, 2004.

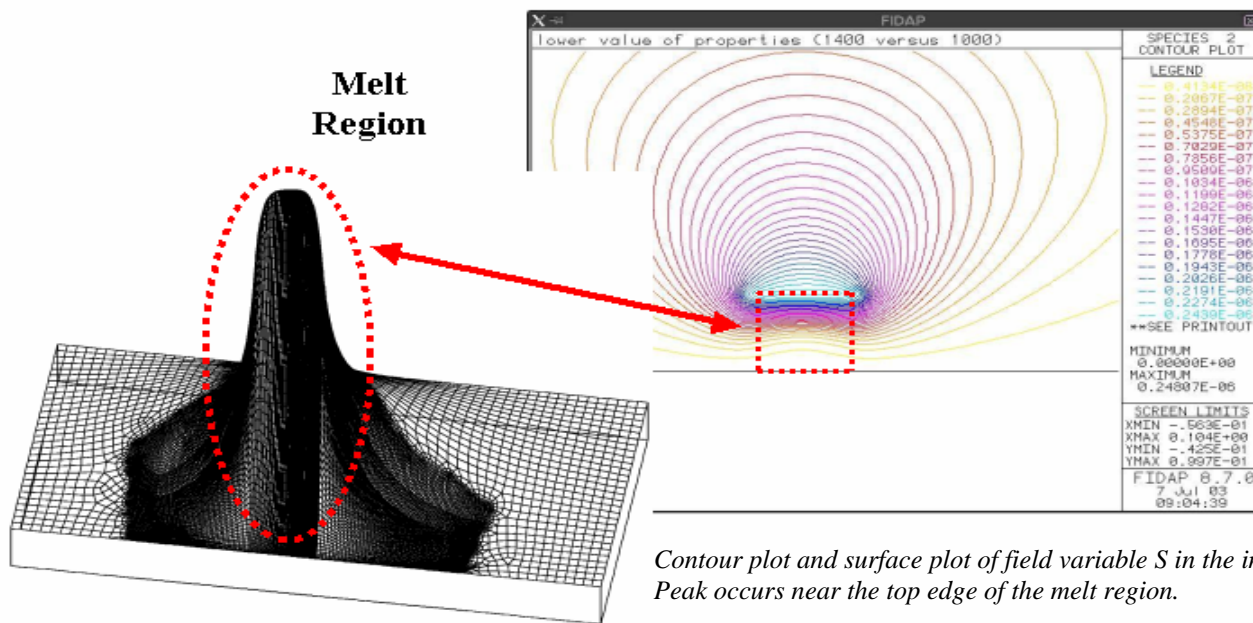
T. Tan, R. Clarksean, Y. Chen, S. Hsieh, and M. Meyer, "Simulating the Induction Heating Process in an Induction Skull Melter for Casting Metallic Fuel," *ICONE-12*, Arlington, VA, April 25-29, 2004.

T. Tan, R. Clarksean, Y. Chen, D. Pepper, and M. Meyer, "Simulation and Analysis for Melt Casting a Metallic Fuel Pin Incorporating Volatile Actinides" *International Mechanical Engineering Congress and Exposition*, Washington, DC, November 16-21, 2003.

X. Wu, R. Clarksean, Y. Chen, D. Pepper, and M.K. Meyer, "An Analysis of the Melt Casting of Metallic Fuel Pins," *International Mechanical Engineering Congress and Exposition*, New Orleans, LA, November 17-22, 2002.

X. Wu, R. Clarksean, Y. Chen, and D. Pepper, "Design and Analysis for Melt Casting Metallic Fuel Pins Incorporating Volatile Actinides," *International Youth Nuclear Congress*, Daejeon, Korea, April 16-20, 2002.

X. Wu, R. Clarksean, and Y. Chen, "Design and Analysis for Melt Casting Metallic Fuel Pins Incorporating Volatile Actinides," *International Congress on Advanced Nuclear Power Plants*, Hollywood, FL, June 9-13, 2002.



Research Staff

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Task 2

Modeling, Fabrication, and Optimization of Niobium Cavities

R.A. Schill, Jr., M.B. Trabia, and W. Culbreth

BACKGROUND

One of the key technologies for the deployment of accelerator-driven transmutation systems is the accelerator itself. Elliptical superconducting niobium cavities are used to increase the efficiency of the high-power accelerators needed to support the transmutation mission.

One of the major sources of energy loss from a superconducting accelerator cavity is a process known as multiple impacting (or “multipacting”) of electrons. This phenomenon limits the maximum amount of energy and power that the niobium cavity can store. As a result, the maximum power available for accelerating the desired charge, as well as the overall performance of the accelerator is reduced. Furthermore, the energy absorbed as a result of multipacting eventually turns into heat. This negatively impacts the performance of both the superconducting cavity and the accelerator.

RESEARCH OBJECTIVES AND METHODS

This project was tasked with examining the impacts of the design and fabrication technologies for these elliptical niobium cavities on their performance. Niobium was selected primarily due to its behavior at low temperatures.

One objective of this study was to experimentally model the fluid flow resulting in the chemical etching of niobium cavities with the aid of a baffle. Numerical analyses tend to show that

the current etching process with a baffle does not uniformly etch the cavity surface. Multiple cavity cell geometries were investigated. Optimization techniques were applied in search of the chemical etching processes, which would lead to cavity walls with near ideal properties.

A Monte Carlo secondary electron microscopy (SEM) code was modified to provide a statistical study of electron impact from Los Alamos National Laboratory (LANL) cleaned niobium samples at near cryogenic temperatures in a UHV environment. A one-of-a-kind secondary electron emission test stand was developed to study, in part, the dynamics of the emitted particles subjected to an electron beam. Coordinating code studies with experiments offers a wealth of knowledge regarding the surface physics of the material that can enhance modeling codes at LANL.

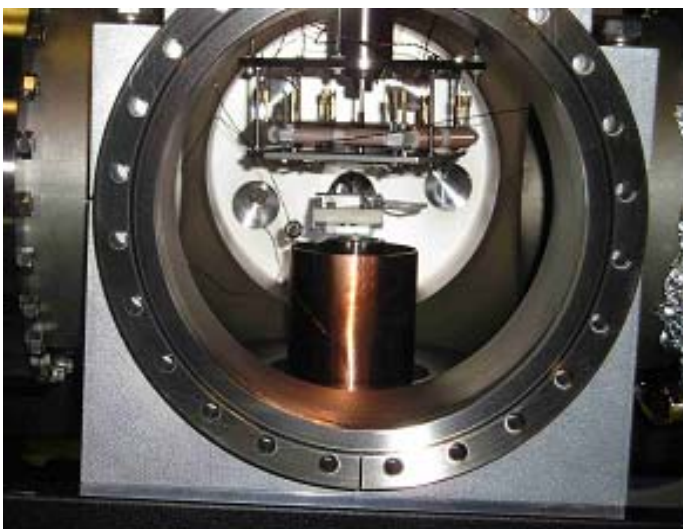
Modeling codes, optimization techniques, and experimentation provided UNLV researchers with a well-rounded study to examine existing and novel niobium cavity designs and cleaning processes for the superconducting radio frequency high-current accelerator.

RESEARCH ACCOMPLISHMENTS

Monte Carlo SEE Code Development and Modifications: A Monte Carlo secondary electron emission code based on the “Single Scatter” approach was obtained from Dr. David Joy of both ORNL and the University of Tennessee. The “Single Scatter” approach follows the primary electron and each generation of secondary electron through the entire cascade. The code was modified to allow for surface layer contaminants in the hopes to verify experimental studies. The code only offers approximate results since the inherent mechanisms internal to the code are valid at higher primary beam energies. A SEE code was used to study the initial particle trajectory conditions of the secondary electron released by the primary electron impacted niobium sample. Results were compared with experiments.

SEE (Secondary Electron Emission) Studies: Niobium samples were cleaned both at LANL and Cornell University and used for experimentation. Two types of cleaning procedures have been used: electro-polishing and buffered chemical polishing. *In situ* pictures of the sample surface were taken with a long-range light microscope for future comparisons.

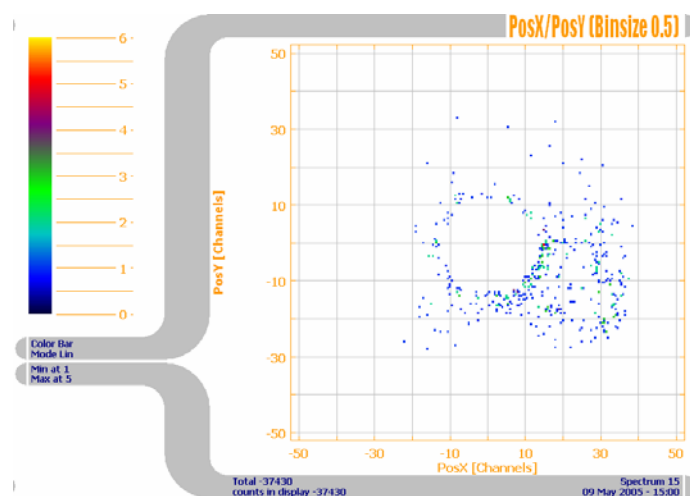
The experimental setup is unique offering further insights to the SEE process not attained elsewhere. Individual electrons are detected and mapped over the detector surface. With the aid of particle tracking codes, knowledge of the final condition of the electron suggests a family of initial particle trajectory conditions of the emitted electron. Using the Monte Carlo SEE code, the family of initial conditions were evaluated. By March



Side view of the secondary electron emission system. The components from top to bottom are: electron gun end, electron beam tube, particle position detector, micro-channel plate stack, business end of the manipulator arm, top of cryostat, and cryostat thermal guard.

2004, many of the components of the experimental study reached UNLV with some assembly accomplished. The first secondary electron emission (SEE) measurement was made from the surface of a Faraday cup in September 2004. In December of 2004, the software for the particle positioning detector was finally up and running. The integrity of the code and detector were fine-tuned and initial experiments were completed by April 2005. Experiments on the surface cleaned samples were completed in May of 2005. Experimental studies were completed on the samples provided by LANL.

Revised Etching Process: The current etching method, which uses a baffle to direct the etching fluid toward the surface of the cavity, partially succeeded in achieving its task. However, flow was restricted to the right half of the cavity with very limited circulation in the left half. An alternative design was proposed and modeled. The exit flow is now parallel to flow inlet. Results show that flow circulation was eliminated. The flow is now closer to the surface of the cavity. Optimization techniques were used to improve this design.



Typical secondary electron emission detected when a 100 ms pulse, 1 keV electron beam impinges on a 30 degree incline, virgin surface of niobium before in situ sample baking. Each pixel represents a spatial bin on the detector. The color of the pixel corresponds to the number of electrons detected at that position. The sample was buffered chemically polished. Single count events have been removed to enhance the scattering tendency.

Developed Flow Visualization System: To confirm the predictions from the fluid flow models used to analyze the etching process, the UNLV team developed and deployed a flow visualization system. A complete experimental setup, including a computer-controlled x-y traverse and digital camera, was assembled. Flow visualization experiments using a plastic prototype of the niobium cavity used dye injection. Dye injection provided quantitative verification that laminar flow exists within the niobium cavities during etching. Additionally, it verified the absence of re-circulation pockets within the cavities.

The etching process and flow visualization process has led to a thesis. The secondary electron emission studies will also lead to a thesis in the summer of 2005. Results are to be presented at the IEEE ICOPS conference in June of 2005 and a referred journal paper is to be submitted during the summer of 2005.

TASK 2 PROFILE

Start Date: June 2001

Completion Date: July 2005

Theses Generated:

Qin Xue, M.S., Mechanical Engineering, "Modeling and Simulation of the Chemical Etching Process in Niobium Cavities," August 2002.

Satish Subramanian, M.S., Mechanical Engineering, "Modeling, Optimization, and Flow Visualization of Chemical Etching Process in Niobium Cavities," May 2004.

Anoop George, M.S. Electrical and Computer Engineering, "Study of Secondary Electron Emission from Niobium at Cryogenic Temperatures," August 2005.

Conference Proceedings:

A. George, R.A. Schill, Jr., R. Kant, and S. Goldfarb, "Secondary Electron Emission from Niobium at Cryogenic Temperatures," International Conference on Plasma Science 2005, Monterey, CA, June 20-24, 2005.

M.B. Trabia, W. Culbreth, S. Subramanian, and T. Tajima, "Optimization of Chemical Etching Process in Niobium Cavities," *Proceedings*, ASME 2004 Design Engineering Technical Conferences and Computers and Information in Engineering Conference, Salt Lake City, UT, September 28 – October 2, 2004.

M. Holl, M. Trabia, and R.A. Schill, Jr., "Optimization of a Five-Cell Niobium Cavity," Sixth International Topical Meeting on the Nuclear Applications of Accelerator Technology, San Diego, CA, June 1-5, 2003.

Q. Xue, S. Subramanian, M. Trabia, Y.T. Chen, and R.A. Schill, Jr., "Modeling and Optimization of the Chemical Etching Process in Niobium Cavities," International Congress on Advanced Nuclear Power Plants, Hollywood, Florida, June 9-13, 2002.

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Task 3

Corrosion of Steel by Lead Bismuth Eutectic

J.W. Farley, A. Johnson, and D.L. Perry

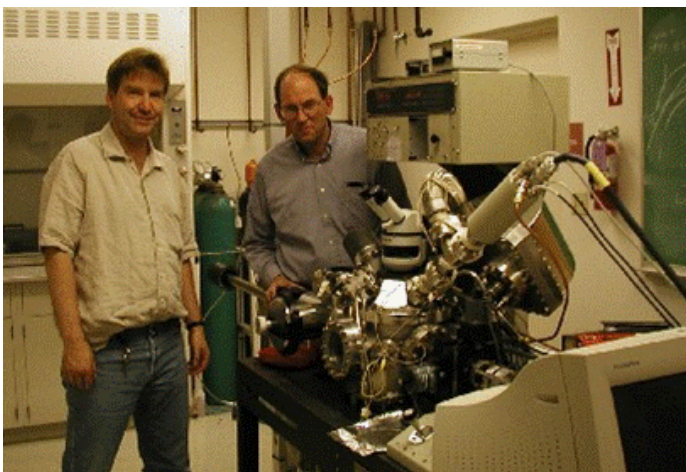
BACKGROUND

There is an active international interest in lead-bismuth eutectic and similar liquid lead systems because of the relevance to the transmutation of nuclear waste, fast reactors, and spallation neutron sources.

Materials in these systems must be able to tolerate high neutron fluxes, high temperatures, and chemical corrosion. For lead bismuth eutectic (LBE) systems, there is an additional challenge because the corrosive behaviors of materials in LBE are not well understood. Most of the available information on LBE systems has come from the Russians, who have over 80 reactor-years experience with LBE coolant in their Alpha-class submarine reactors. The Russians found that the presence of small amounts of oxygen (on the order of parts per million) in the LBE significantly reduced corrosion. However, a fundamental understanding and verification of its role in the corrosion of steels is incomplete.

RESEARCH OBJECTIVES AND METHODS

This research program has analyzed various steel samples that have been exposed to lead bismuth eutectic as part of the national program to develop LBE and allied technologies. The goal of this research is to understand the basic science of corrosion in the steel/LBE system. This information will be paramount in developing engineering efforts to control, avoid, and/or minimize the effect of corrosion of steels by LBE in transmuter and LBE systems. Additionally, this program provides UNLV researchers with hands-on experience that will be crucial in developing the UNLV molten metal program.



Professors Allen Johnson and John Farley next to an X-ray Photoelectron Spectrometer.

Investigators performed post-experiment testing and analysis on steel samples that have been exposed to lead bismuth eutectic. Surface analysis techniques were employed that included Scanning Electron Microscopy (SEM), Energy Dispersive X-ray (EDAX) spectroscopy, X-ray Photoelectron Spectrometry (XPS), and laser Raman spectrometry.

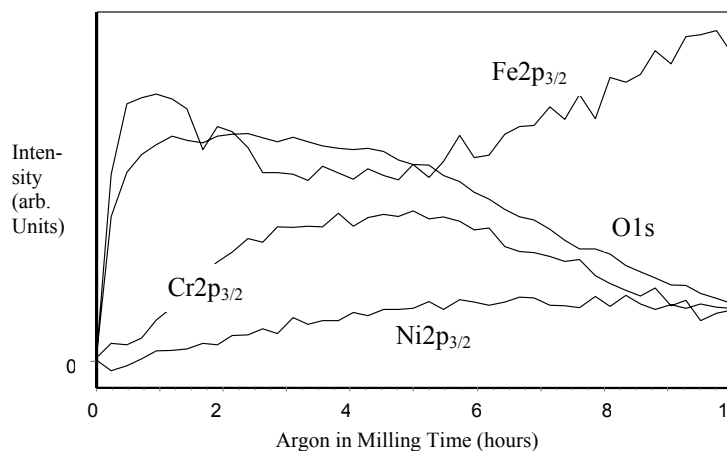
These techniques, applied to the steel surface, have probed the surface morphology, elemental composition, and oxidation states as a function of position. Chemical alterations and resulting chemical species were studied at the steel surface. Additionally, the experimental facilities at the Advanced Light Source (Lawrence Berkeley National Laboratory) and the Advanced Photon Source (Argonne National Laboratory) were used to characterize the systems. This allowed spectroscopic characterization of the stainless steel before and after interaction with LBE to determine its composition.

RESEARCH ACCOMPLISHMENTS

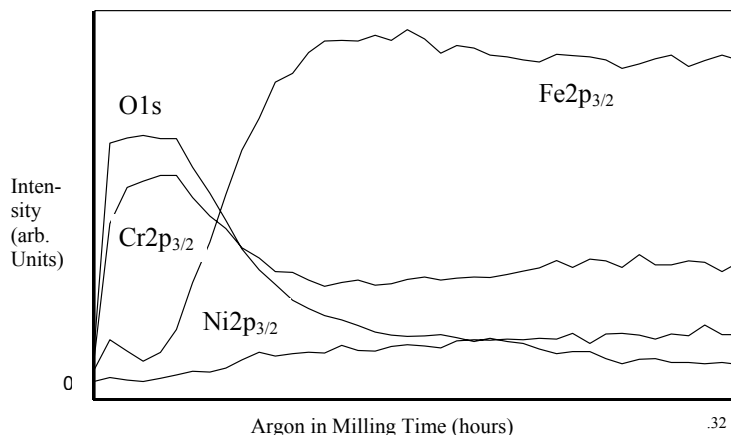
Several samples were compared having the same or similar compositions (standard nuclear grade 316/316L) but different surface preparation, including cold-rolled, annealed and a special low-corrosion treatment, "D-9." The cold-rolled sample had an order of magnitude less corrosion (i.e., both lower oxidation and less weight change) than the annealed sample.

Sputter depth profiling of the exposed annealed sample and cold-rolled sample showed a marked difference in oxide layer composition between the annealed and cold-rolled sample. The annealed sample showed a complex oxide structure (iron oxide over chromium/iron oxide mixtures) of tens of microns thickness, while the cold-rolled sample was covered with a simple, primarily chromium oxide layer approximately one micron thick. Interestingly, the D-9 material behaved more like the annealed than the more resistant cold-rolled material. In addition to these studies of 316/316L steel, other compositions of steel such as HT9 were also studied. These studies show the importance of surface preparation in resistance to corrosion by LBE.

Another alloy studied in the IPPE series was EP823, an alloy similar to HT9 but with added silicon to improve corrosion resistance. A study of silicon in iron was undertaken to investigate the role of silicon in steels for LBE service. A series of silicon-containing iron samples were examined that were exposed to LBE at INL. Several unique features were observed: at low silicon concentrations in the starting alloy, the silicon was found as a silicate (SiO_3^{2-}). As the concentration of silicon increased in the starting alloy, a layer containing silica (SiO_2) was found also. Under the oxide layer, the silicon concentration in the metal was found to be decreased by approx-



Sputter Depth Profile of annealed 316/316L stainless steel sample. Note iron oxide at the surface.



Sputter Depth Profile of cold-rolled 316/316L stainless steel sample. Note chromium oxide at the surface.

-mately 30%. These were model systems, and the oxide layers that formed were not very protective. In all cases, pockets of LBE were found underneath the oxide layer, potentially corroding the steel.

TASK 3 PROFILE

Start Date: June 2001

Completion Date: May 2004

(This work is continued as Task 18, see pages 40-41.)

Thesis Generated:

Daniel Koury, M.S., Physics Department, "Investigation of the Corrosion of Steel by Lead-bismuth Eutectic (LBE) Using Scanning Electron Microscopy And X-ray Photoelectron Spectroscopy," December 2002.

Journal Article:

A.L. Johnson, D. Parsons, J. Manzerova, D.L. Perry, D. Koury, B. Hosterman, and J.W. Farley, "Spectroscopic and Microscopic Investigation of the Corrosion of 316/316L Stainless Steel by Lead-Bismuth Eutectic (LBE) at Elevated Temperatures: Importance of Surface Preparation," *J. Nuclear Materials*, **328** (2004) 88-96.

Conference Proceedings:

"Mechanisms of Lead-Bismuth Eutectic Corrosion Chemistry involving Stainless Steels in Nuclear Reactor Cooling Systems," Annual Meeting of the American Chemical Society, Anaheim, CA, March 29-31, 2004.

A. Johnson, D. Parsons, J. Manzerova, D. Koury, B. Hosterman, D.L. Perry, and J.W. Farley, "Surface Studies of the High Temperature Corrosion of Stainless Steel by Oxygen Controlled Lead-Bismuth Eutectic," American Vacuum Society, Baltimore, MD, Nov. 2-7, 2003.

"Chemical Species Involved in High Temperature Corrosion Resulting from the Interaction Between Stainless Steel and Lead-Bismuth Eutectic," 38th Western Regional Meeting of the American Chemical Society, Long Beach, CA, October 15-18, 2003.

A.L. Johnson, D. Parsons, J. Manzerova, D.L. Perry, D. Koury, B. Hosterman, and J.W. Farley, "Surface Studies of the Corrosion of Stainless Steel by Lead Bismuth Eutectic: Surface Preparation Effects on 316 Stainless Steels," American Nuclear Society Summer Meeting, San Diego, CA, June 1-5, 2003.

D. Koury, A.L. Johnson, D.L. Perry, and J.W. Farley, "Investigation of Corrosion of Steel by Lead Bismuth Eutectic," ANS Topical Mtg. on Accelerator Applications, AccApp/ADTTA01, Reno, NV, Nov. 2001.

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Task 4

Environment-Induced Degradation and Crack-Growth Studies of Candidate Target Materials

A.K. Roy

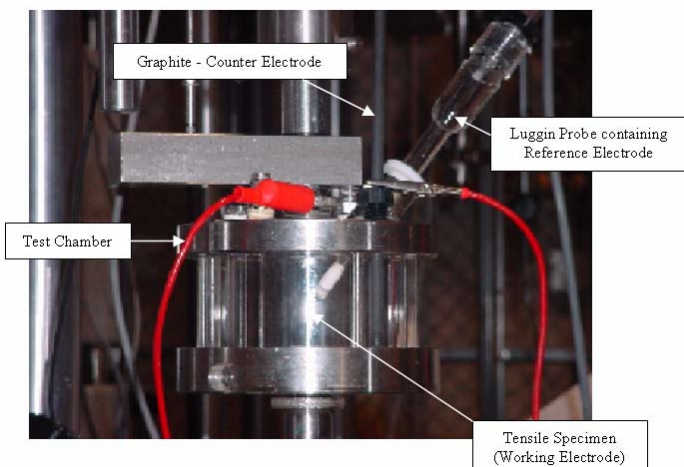
BACKGROUND

The primary objective of this task was to evaluate the effects of environmental and mechanical parameters on environment-induced degradations of candidate target structural materials for applications in spallation-neutron-target systems. The materials selected for evaluation and characterization were martensitic stainless steels including Alloys HT-9, EP-823, and 422.

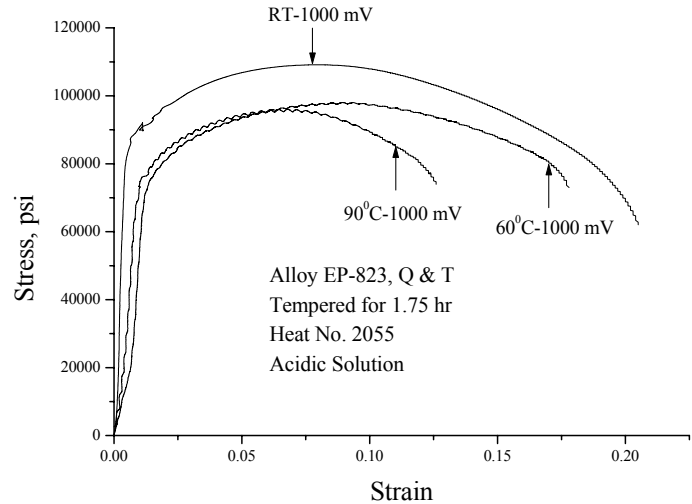
Accelerator-driven transmutation systems involve bombarding a target material such as molten lead-bismuth-eutectic (LBE) by a proton beam, thereby producing neutrons. The molten LBE target will be contained in a subsystem structural container made of a suitable material such as Alloys HT-9, EP-823, and 422. During the transmutation process, the target structural material may become susceptible to different types of environment-induced degradations such as stress corrosion cracking (SCC), hydrogen embrittlement (HE), and localized (pitting and crevice) corrosion. While the performance of these candidate materials in the presence of a molten LBE is yet to be evaluated, substantial work has been performed in this task to evaluate the corrosion behavior of these alloys in aqueous environments of interest. These baseline data can eventually be utilized to compare them to those yet to be generated in the molten LBE environment.

RESEARCH OBJECTIVES AND METHODS

This investigation was focused on the evaluation of the susceptibility of all three martensitic alloys to SCC, HE, and localized corrosion in neutral and acidic aqueous environments at ambient and elevated temperatures. State-of-the-art experimental techniques including constant-load (CL), slow-strain-rate (SSR), and cyclic potentiodynamic polarization (CPP) were employed to evaluate these corrosion phenomena.



Controlled Potential Test Setup



Stress vs Strain under Controlled Potential.

The susceptibility of these alloys to HE was evaluated by applying cathodic potential while the test specimens were loaded in tension by the SSR method. Optical microscopy and scanning electron microscopy (SEM) were used to analyze the metallurgical microstructures and fractography, respectively of the tested specimens.

RESEARCH ACCOMPLISHMENTS

The significant results derived from this task are summarized as follows:

- No failures were observed in smooth specimens of Alloys EP-823 and 422 in the neutral solution when tested at CL. However, Alloy HT-9 showed failure in the 90°C neutral solution at an applied stress (σ_a) of 112 ksi.
- All three alloys exhibited failure in the 90°C acidic solution at 95% of their YS values. Alloys HT-9 and 422 also showed failures at σ_a of 90 and 85% of their YS values, but no failure was observed with Alloy EP-823 at stresses below 0.95 YS.
- The magnitudes of the threshold stress (σ_{th}) for cracking for Alloys EP-823, HT-9 and 422 were 100, 95, and 98 ksi (689, 655, and 676 MPa), respectively based on CL testing in the 90°C acidic solution. The presence of a notch in the test specimen reduced the σ_{th} values in all three alloys.
- The results of SSR testing in the acidic solution involving smooth specimens showed gradual reduction in ductility parameters (percent elongation - %El and percent reduction in area-%RA), time-to-failure (TTF), and true failure stress (σ_f) with increasing temperature, indicating a synergistic effect of pH and temperature in enhancing the cracking susceptibility. The presence of a notch in the specimen produced enhanced SCC susceptibility due to the stress concentration. However, the σ_f value was increased due to plastic constraint resulting

from triaxial stress field at the notch.

- The magnitude of %El, %RA, TTF, and σ_f was reduced under an applied potential of -1,000 mV (Ag/AgCl) compared to those obtained without an applied potential.
- The failure mode at the primary fracture face of the specimen tested in the neutral solution, determined by SEM, was characterized by dimpled microstructure, indicating ductile failures. However, intergranular and/or transgranular brittle failures were observed in the acidic environment.
- Secondary cracks with branching were observed by optical microscopy on all three tested materials along the gage section of the specimens tested in the acidic solution.

TASK 4 PROFILE

Start Date: June 2001

Completion Date: December 2004

Theses Generated:

Ramprashad Prabhakaran, M.S., "Environment-Induced Degradations in a Target Structural Material for Transmutation Applications," August 2004.

Sudheer Sama, M.S., "Embrittlement and Localized Corrosion in Alloy HT-9," August 2004.

Phani P. Gudipati, M.S., "Stress Corrosion Cracking Resistance of Martensitic Stainless Steels for Transmutation Applications," December 2004.

Mohammad K. Hossain, Ph.D., "Stress Corrosion Cracking and Hydrogen Embrittlement of Martensitic Alloy EP-823," December 2004.

Venkataramakrishnan Selvaraj, M.S., "Environment Assisted Cracking of Target Structural Materials under Different Loading Conditions," December 2004.

Journal Articles:

A.K. Roy and M. K. Hossain, "Cracking of Martensitic Alloy EP-823 under Controlled Potential," *Journal of Materials Engineering and Performance*, ASM International, (In Review).

A.K. Roy, M. K. Hossain, R. Prabhakaran and S. Sama, "Environment-Assisted Cracking of Structural Materials under Different Loading Conditions," *Corrosion*, NACE International, April 2005, Vol. 61, No. 4, pp. 364-370.

A.K. Roy, R. Prabhakaran, M. K. Hossain and S. Sama, "Stress Corrosion Cracking of Nuclear Transmutation Structural Materials," *Materials Performance*, NACE International, September 2004, Vol. 43, No. 9, pp. 52-56.

Conference Proceedings:

A.K. Roy, and M. K. Hossain, "Environment Induced Embrittlement of Martensitic Stainless Steel for Transmutation Applications," *Corrosion 2005*, NACE International, Houston, TX, April 2005.

A.K. Roy, Phani P. Gudipati, Venkataramakrishnan Selvaraj, "Environment Degradation of Martensitic Stainless Steels for Transmutation Applications," *MS&T 2004*, New Orleans, LA, September 26-29, 2004.

A.K. Roy, R. Prabhakaran, "Stress Corrosion Cracking of Type 422 Stainless Steel for Transmutation Applications," *International Youth Nuclear Congress (IYNC) 2004*, Toronto, Canada, May 9-13, 2004.

R. Prabhakaran and A.K. Roy, "The Effect of Environmental and Mechanical Variables on Stress Corrosion Cracking of Martensitic Stainless Steels for Transmutation Applications," *ICONE-12*, Student Paper Competition, Arlington, VA, April 25-29, 2004.

A.K. Roy, M. K. Hossain, R. Prabhakaran, S. Sama, V. Selvaraj, P.P. Gudipati, "Stress Corrosion Cracking of Target Materials for Transmutation Applications," *Corrosion 2004*, NACE International, New Orleans, LA, March 28-April 1, 2004.

A.K. Roy, R. Prabhakaran, "Characterization of Environment-Induced Degradation in Type 422 Stainless Steel," *TMS 2004*, Charlotte, NC, March 14-18, 2004.

A.K. Roy, R. Prabhakaran, M. K. Hossain, S. Sama, V. Selvaraj, P.P. Gudipati, "Effect of Environmental Variables on Cracking of Martensitic Stainless Steels under Different Loading Conditions," *ANS Meeting-Global 2003*, New Orleans, LA, November 16-20, 2003.

A.K. Roy, R. Prabhakaran, M. K. Hossain, S. Sama, V. Selvaraj, P.P. Gudipati, "Environmental Effects on Materials For Nuclear Applications," *MS&T 2003*, Chicago, IL, November 9-12, 2003.

A.K. Roy, S. Sama, R. Prabhakaran, M. K. Hossain, "Cracking of Martensitic Stainless Steels under Applied Electrochemical Potential," 204th Meeting of the Electrochemical Society (ECS), Abstract No. 1255, Orlando, FL, October 12-17, 2003.

A.K. Roy, R. Prabhakaran, M. K. Hossain, S. Sama, B. J. O'Toole, "Environment-Induced Degradation of Spallation Target Materials," *ANS Meeting, AccApp'03*, San Diego, CA, June 1-5, 2003.

A.K. Roy, M. K. Hossain, B. J. O'Toole, "Stress Corrosion Cracking of Martensitic Stainless Steel For Transmutation Applications," *The 10th International High-Level Radioactive Waste Management Conference*, Las Vegas, NV, March 30-April 3, 2003.

R. Prabhakaran, "Stress Corrosion Cracking of Type 422 Stainless Steel For Applications in Spallation-Neutron-Target Systems," *Spallation Neutron Source (SNS)-JINS-NICEST 2003*, Oak Ridge, TN, March 12, 2003.

A.K. Roy, M.K. Hossain, and B.J. O'Toole, "Stress Corrosion Cracking of Martensitic Stainless Steel for Transmutation Applications," *International High-Level Radioactive Waste Management Conference*, Las Vegas, NV, Sept. 2002.

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Task 5

Modeling Corrosion in Oxygen Controlled LBE Systems with Coupling of Chemical Kinetics and Hydrodynamics

S. Moujaes and Y. Chen

BACKGROUND

The corrosion of structural materials is a major concern for the use of lead-bismuth eutectic (LBE) systems for nuclear applications such as in transmuter targets or fast reactors. Corrosion in liquid metal systems can occur through various processes, including, for example, dissolution, formation of inter-metallic compounds at the interface, and penetration of liquid metal along grain boundaries. Predicting the rate of these processes depends on numerous system operational factors: temperature, system geometry, thermal gradients, solid and liquid compositions, and velocity of the liquid metal, to name a few. Corrosion, along with mechanical and/or hydraulic factors, often contributes to component failure.

The goal of this project is to develop a corrosion model that combines the chemical kinetics and hydrodynamics in the system to predict corrosion rates. In this effort, these models will be developed for the Delta test loop at Los Alamos National Laboratory (LANL) and a theoretical LBE accelerator target system. The resulting models will be predictive tools that can be validated with corrosion test data and used to systematically design tests, interpret the results, and provide guidance for optimization in LBE system designs.

RESEARCH OBJECTIVES AND METHODS

There are two subtasks to this research. The first subtask develops the necessary tools to predict the levels of oxygen and corrosion products close to the boundary layer using Computational Fluid Dynamics (CFD) modeling. The second subtask predicts

the corrosion process kinetics between the LBE and structural materials by incorporating pertinent information from the first subtask.

STAR-CD software was used to model the corrosion and precipitation rates in the LBE loop. This allowed researchers to compare the theoretical analysis with available experimental results. The surface corrosion analysis is being developed as a user supplied subroutine to STAR-CD. The information obtained from this analysis theoretically predicts likely locations for corrosion and precipitation along the axial lengths of the test loop.

The first subtask involved performing a series of parametric runs. Models prepared from the previous year were used as guides for the parametric studies. Variables investigated included the average eutectic flow velocity, average mean bulk eutectic flow, inlet temperatures, and average inlet oxygen concentrations in the three geometries: a straight flow section, an elbow bend, and a tee section. The thermal-hydraulics study involved using a 3-D CFD code simulation to obtain averaged values of stream-wise velocity, temperatures, and oxygen and corrosion product concentrations at various axial locations close to the walls of several partial loop sections within the LBE loop. The oxygen and corrosion products inside the test loop were simulated to participate in chemical reactions with the eutectic fluid as it diffused towards the walls. Details of the geometry of these loops will be obtained from scientists at LANL. These values acted as a set of starting boundary conditions for the second task.

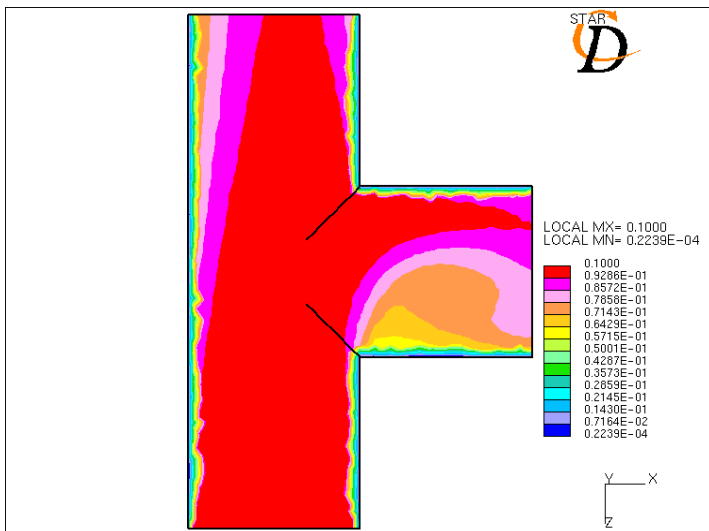
The second subtask focused on the kinetics of the dissolution/deposition process as a function of temperature, flow velocities, dissolved metal concentrations, oxygen potentials of the system, the kinetics of film formations in the presence of oxygen, and the kinetics of metal transport through the oxidized surface film.

RESEARCH ACCOMPLISHMENTS

Geometries and flow conditions similar to experimental results in the literature were set up and used to benchmark the models assembled using the STAR-CD software. Test case studies indicated that the outcome from STAR-CD was correct and that numerical modeling is applicable to the research in this problem.

Using these models, concentration flux profiles were obtained for both laminar and turbulent profiles in a straight pipe. This information was then used for the chemical kinetics analysis for corrosion on the inside walls of the LBE loop.

Several CFD runs were made to simulate flow in pipe fittings. These include sudden contraction, sudden expansion and a T-joint. Testing of a new turbulent model was also performed using



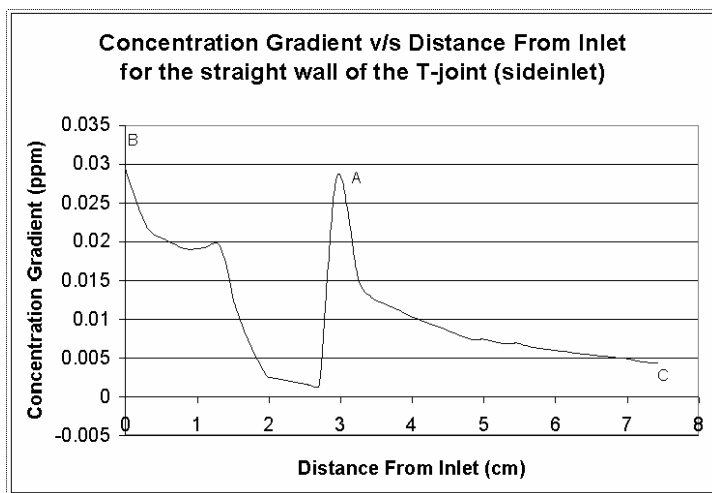
Concentration profile for T-joint at $Re = 200,000$.

the k- ϵ Chen model which works better with high Re number flows and predicts some of the peculiar flow features relevant to sudden expansions where eventually vortex generation is expected at the backward step.

A user subroutine was developed that simulated the corrosion/precipitation processes and predicted their maximum/minimum location in a typical LBE loop. A chemical reaction subroutine dealt with surface chemistry. The Arrhenius Equation was used to calculate the reactant reaction rate but some constants and coefficients used in calculating chemical reaction rate were updated using some empirical data found in chemical reaction research papers and textbooks.

The location in the loop with the highest concentration occurred in the baffle cell which is adjacent to the iron surface while the area with lowest concentration occurs around the central line of the pipe. It can be inferred that after Fe_3O_4 is formed, it diffuses to the fluid area close to the central line of pipe. But, overall, the concentration value was very low.

Similar to the concentration gradient, the area with the highest temperature occurs in the baffle cell which is adjacent to iron surface while the area with lowest temperature occurs around the central line of the pipe. It is obvious, based on the model, that heat was transferred from inner wall to central area of the pipe due to the setting of constant heat flux boundary conditions in the baffle cells.



Concentration gradient versus distance from the inlet for the straight wall.

The chemical reaction model subroutine worked well and this simple CFD model roughly simulated the chemical reaction, diffusion, and heat transfer condition inside the LBE piping. Since the subroutine works well, it can be used in much more complex modeling.

TASK 5 PROFILE

Start Date: August 2001

Completion Date: August 2004

Theses Generated:

Chao Wu, M.S., Mechanical Engineering, "Study of Geometry Effects on Local Corrosion Rates for LBE Loop," July 2003.

Kanthi Dasika, M.S., Mechanical Engineering, "Chemical Kinetics and Thermal Hydraulics of Lead Bismuth Flow Loops," December 2003.

Narain Armbya, M.S., Mechanical Engineering, "CFD Analysis of 3-D Thermal Hydraulics Flow Effects on Wall Concentration Gradient Profiles for LBE Loop Fittings," December 2004.

Conference Proceedings:

C. Wu, K. Dasika, Y. Chen, S. Moujaes, J. Zhang and N. Li, "Study of Geometry Effects on Local Corrosion Rates for LBE Loop," ANS National Conference, San Diego, CA, June 1-5, 2003.

S. Moujaes, Y. Chen, K. Dasika, C. Wu, N. Li, and J. Zhang, "Simulation Considerations in Lead-Bismuth Transmutation Loops: Corrosion Concentration, velocity and Temperature Profiles of LBE Loops," NURETH-10, South Korea Oct. 5-9, 2003.

K. Dasika, C. Wu, S. Moujaes, and Y. Chen, "Modeling of Oxygen Controlled Surface Reaction Kinetics and Hydrodynamics," International Youth Nuclear Congress, Seoul, South Korea, April 2002.

K. Dasika, C. Wu, S. Moujaes, and Y. Chen, "Numerical Modeling of Lead Oxidation in Controlled Lead Bismuth Eutectic Systems: Chemical Kinetics and Hydrodynamic Effects," ICAPP Conference, Hollywood Florida, ANS, June 2002.

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Task 6

Neutron Multiplicity Measurements of Target/Blanket Materials

D. Beller

BACKGROUND

To optimize the performance of accelerator-driven sub-critical (ADS) transmutation systems, engineers will need to design the system to operate with a neutron multiplication factor just less than that of a critical, or self-sustaining, system. This design criterion requires particle transport codes that instill the highest level of confidence with minimal uncertainty, because larger uncertainties in the codes require larger safety margins in the design and result in a lower efficiency of the ADS transmuter. For current design efforts in the U.S., a Monte Carlo particle transport code MCNPX is used to model neutron production and transport for spallation neutron systems.

While providing a very useful research and modeling tool, uncertainties in MCNPX and associated data libraries, particularly at higher energies, require engineers to increase the safety margin in the designs of the ADS transmuter. Much of the uncertainty associated with MCNPX is thought to be due to the escape of multiple high-energy particles from the target (multiple scattering), along with uncertainties in the predictions of source term volume measurements. Determining a reliable method that measures, validates, and benchmarks the calculations of such a volumetric source term is necessary.

The primary goal of this research is to develop a detector system for the measurement of neutron production in spallation targets, to test the system in a variety of calibrated beam lines, and to produce precise, position-sensitive measurements of the volumetric neutron source term to provide data for validation of ADS design codes.

RESEARCH OBJECTIVES AND METHODS

A prototype modular neutron detector system with 64 ^3He gas counting tubes was developed in conjunction with collaborators at the V.G. Khlopin Radium Institute (KRI) in St. Petersburg, Russia to measure the neutron multiplicity of scaled lead accelerator targets. The system, which has been named the Neutron Multiplicity Detector System (NMDS) was fabricated by KRI and shipped to UNLV. Its modularity allows it to be configured for a variety of experiments to measure neutron multiplicity from different sources: protons, electrons, high-energy neutrons, or even cosmic particles such as muons.

The NMDS is constructed from lead bricks that may be arranged in a 30 x 30 x 30 cm cubic configuration for cosmic ray measurements or as an elongated accelerator target, either 15 x 15 x 120 cm or 20 x 20 x 60 cm (smaller arrangements are also possible). This system may be used to measure neutron production in a variety of configurations, on a variety of targets, with a variety of source particles, and over a range of energies (10 to 800 MeV) to produce a large data base that may be used to validate neutron multiplicity predictions.



View of detector system aligned with accelerator vacuum tube and window. The beam height had not been adjusted in this photograph. The AmBe source can be seen in the opening in the polyethylene bricks of the NMDS.

Time-dependent measurements of neutron production in the NMDS were intended to provide a systematic set of precise data that will enable direct comparison with code calculations, such as MCNPX and its accompanying data libraries. Comparison of results from the NMDS with calculations may decrease uncertainties. In addition, discrepancies that were discovered with this system could contribute to the improvement of the codes and data libraries. Improved models of beam line experiments, accelerator targets, and detector designs should result from these code improvements.

RESEARCH ACCOMPLISHMENTS

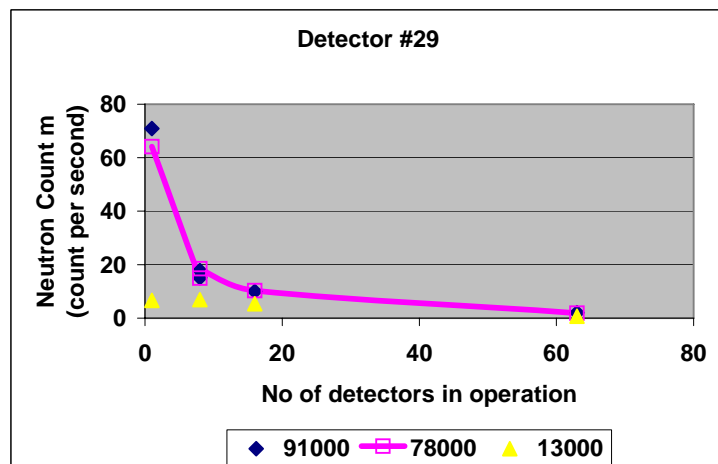
To evaluate its usefulness for measurement of spallation neutrons, the NMDS was transported to the Idaho Accelerator Center at Idaho State University where it was used in conjunction with an accelerator to determine its performance. This involved disassembling the system, packing it in its shipping crates, transporting it to ISU, reassembling it, and conducting a series of accelerator-driven experiments. At the IAC the electron beam was pointed at one face of the Pb (see picture above). After the experiments were completed, the system was returned to UNLV and reassembled there.

Several different cubic and rectangular configurations were examined, and all configurations were modeled in MCNPX prior to the experiments. The rectangular configurations were created in anticipation of conducting neutron multiplicity experiments on high-energy proton linear accelerators (linac) at the Los Alamos Neutron Science Center or at Brookhaven National Laboratory.

An AmBe source with a neutron production rate of $2500 \pm 10\%$ n/s was placed against the face of the Pb in all 5 configurations to measure the overall efficiency of the system. This weak source exceeded the counting capacity of the NMDS, such that its efficiency was reduced to 3.5% compared to earlier values at UNLV of 20-30% with a source strength of ~ 600 n/s.

An attempt to de-tune the accelerator was made by adjusting the electron beam to low current at frequencies of 15, 30, and 120 Hz. At 120 Hz, the deadtime of the detectors caused the system to acquire data for only 20-25% of the pulses. After the initial test runs, the frequencies were restricted to 15 Hz and 30 Hz for data acquisition, which allowed data to be acquired for 82-99% of the pulses received from the accelerator. However, excessive deadtime continued to reduce the counting efficiency. All results from the ISU-IAC accelerator-driven experiments were influenced by a count-rate limitation that is inherent in the NMDS hardware and software.

In an effort to determine system contributions to dead time, a deadtime measurement experiment was conducted at the Remote Sensing Laboratory (RSL) of the Nevada Test Site. The measurement was conducted using a cubic configuration and 64 detectors arranged in four banks of 16. Two ^{252}Cf neutron sources of 13,000 and 78,000 neutrons/second were used to perform two-source deadtime measurements. The data was analyzed and the deadtime coefficients were determined. Results indicated that the performance of individual detectors depends upon the number of detectors operating as well as the source strength (see figure below).



Performance of Detector #29 versus number of detectors in operation and source strength. The combined strength of the two sources is 91,000 n/s. The number of detectors were 1, 8, 16, and 64.

ACADEMIC YEAR HIGHLIGHTS

- ◆ T. Beller visited the ISU Idaho Accelerator Center and the NTS Remote Sensing Laboratory to work with others to conduct experiments with the NMDS. The NMDS was used with a 30-MeV Fast Pulse Linac electron accelerator at the IAC and with two ^{252}Cf sources at the RSL.
- ◆ S. Patil and T. Beller presented a poster at the Eighth Information Exchange Meeting on Actinide and Fission Product Partitioning & Transmutation, 9-11 November 2004, Las Vegas, NV. An accompanying paper, "The UNLV Neutron Multiplicity Detector System," was accepted for publication in the conference proceedings to be published by the OECD-NEA.
- ◆ S. Patil received a second place award in the Accelerator Applications track for her presentation of "Neutron Detector Characteristics in Deadtime Experiments," ANS Student Conference, Columbus, Ohio, April 15, 2005.

The individual detectors were determined to have a deadtime coefficient of a few ms, which would indicate a capability of the total system to count several thousand neutrons per second. However, the system has never counted more than 200 n/s, even with strong neutron sources. Each system component contributes to deadtime: ^3He tubes, pre-amplifiers, signal processing boxes which support 8 detectors each, and the "special computer." In the final analysis, however, these experiments at ISU-IAC and NTS-RSL demonstrated that the performance of the system is critically limited because the "special computer" simply cannot process the data throughput during high count rates. In contrast, 50 or more counts from were measured from cosmic neutrons in a single 256 μs burst, a rate of 2×10^5 counts per second, but these events never happen even once a second. As a consequence of these experiments, a modern data acquisition system is being acquired that will support the maximum performance of each detector and all the detectors combined.

FUTURE WORK

The experiments conducted at the ISU-IAC and the NTS-RSL provided a much better understanding of the capabilities and limitations of the NMDS. The system is severely limited by deadtime. Subsequent to this determination, new data acquisition hardware and software were ordered for modification of the NMDS to count at much higher rates. After the system is modified, it may be tested with electron and proton accelerators. In addition, its use will be investigated in other projects, such as nuclear materials protection, control, and accountability for homeland security and proliferation resistance.

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Task 7

Development of Dose Coefficients for Radionuclides Produced in Spallation Targets

P.W. Patton and M.J. Rudin

BACKGROUND

Ensuring the safety of workers at accelerator-driven nuclear facilities is paramount before these systems can be deployed for nuclear transmutation or any other mission. Spallation neutron sources produce as many as 660 rare radionuclides in either the target or blanket during the spallation process. No data exists for many of these radionuclides in the current radiation protection guidelines and standards. This research program seeks to address this problem through generating internal and external dose coefficients (DCs) for these “new” isotopes.

Dose coefficients permit simple determination of radiation dose associated with various exposure scenarios, and ultimately permit radiation safety personnel to assess the health risks to workers in a nuclear facility. Specifically, radiation safety personnel use dose coefficients to determine the radiation dose incurred to a tissue or organ system from a given exposure. These parameters are often expressed in terms of Annual Limits on Intake (ALIs) and Derived Air Concentrations (DACs).

RESEARCH OBJECTIVES AND METHODS

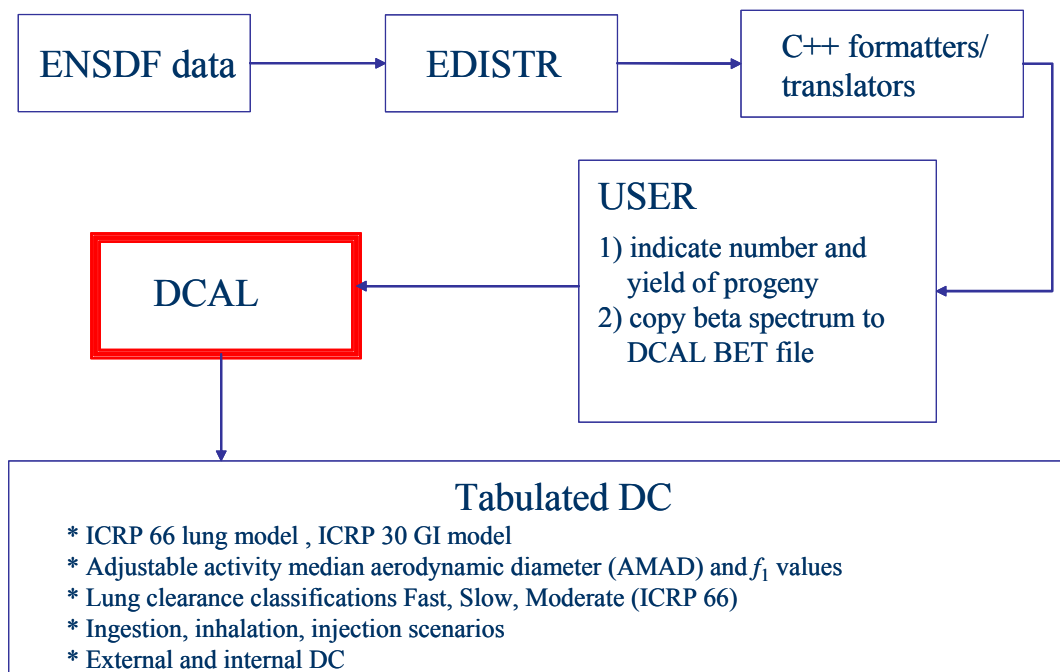
Results from this study will be used to produce ALIs and DACs for these rare radionuclides created by spallation target systems that are not included in Federal Guidance Report (FGR) No. 11. Additionally, DCs developed will augment the radiological data in Publica-

tions 68 and 72 of the International Commission on Radiological Protection (ICRP), contributing to the safe operation of accelerator-driven nuclear systems in the United States and abroad.

A Dose Coefficient Working Group was established in 2001 (the first year of the project) to direct and oversee consortium activities. Representatives from the Dose Coefficient Working Group developed and verified a methodology to determine internal and external dose for select radionuclides. The first step involved obtaining radiological data from the ENSDF nuclear physics database developed at Brookhaven National Laboratory. Data collected included decay modes, decay energy levels, and radiation energies and intensities.

The DC working group prioritized a list of radionuclides projected to be released via air emissions or in the inventory of a mercury target following a lengthy irradiation period. Only radionuclides with a half-life greater than one minute were considered. These 81 radionuclides were then categorized into three distinct categories, based on half-life, available information, and other technical factors.

All Category 2 radionuclides were investigated to determine which database was most current. However, this task was not straight forward and thus both databases were used to calculate all radionuclides that had complete data. Dose coefficients were then generated for the Category 2 radionuclides using both



Dose Coefficient Working Group Methodology Flow Sheet. The ENSDF code is used to obtain nuclear physics data. The EDISTR code prepares the data for input into the dose calculation code DCAL.

ENSDF and NUBASE. The results were compared and showed good agreement. Metabolic models and data from ICRP publications (30 and 66) were applied in order to use the best technology available and to maintain consistency with current standards. In accordance with FGR No. 11, dose coefficients were evaluated for an adult male with the target tissues of gonads, breast, lung, red marrow, bone surface (endosteum), thyroid, remainder, and total committed effective dose equivalent (this considers total dose incurred to specific organs or tissues with respect to radiation type over a period of 50 years). Following determination of these variables, values of ALIs and DACs were then calculated for each radionuclide.

The consortium investigated the competing databases to determine the most appropriate one to use for dose coefficient calculations. However, conflicting data made it unclear which was better suited for this task, therefore the previously calculated coefficients were reported. Additionally, time was devoted to trying to acquire missing nuclear data for radionuclides in category three. Currently, the consortium believes large scale accelerator driven experiments are needed to accomplish this goal.

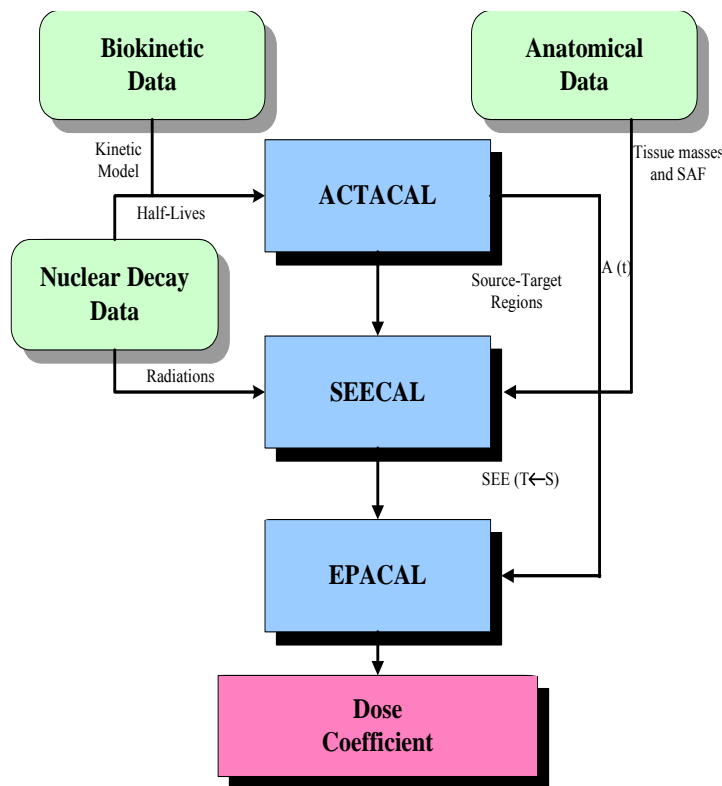
Several of the radionuclides first investigated lack the required nuclear data to calculate dose coefficients (Category 3 radionuclides). The extension of the project has targeted investigating the feasibility of producing these rare radionuclides using the linear accelerator located on Idaho State University's campus. A meeting with Derek Jokisch, David Peterson, and Rich Brey was conducted in January 2005 to discuss the possibility of producing the missing radionuclide data. Much concern was noted on the feasibility of this, therefore an approach that investigates the possible error associated with calculating dose coefficients without the missing electron capture files is being developed.

RESEARCH ACCOMPLISHMENTS

The research consortium comprised of representatives from several universities and national laboratories has successfully generated internal and external dose conversion coefficients for twenty radionuclides produced in spallation neutron sources. These dose coefficients fill data gaps exist in Federal Guide Report No. 11 and in Publications 68 and 72 of the International Commission on Radiological Protection (ICRP), and two articles containing the data have been accepted for publication in the Journal of Health Physics. Currently, more nuclear data is needed for the rare radionuclides produced from a mercury target. While attempting to develop a workable plan to acquire this missing data, Q-value discrepancies are being investigated.

ACADEMIC YEAR HIGHLIGHTS

- ♦ Journal article submitted by A. Arndt, J. Shanahan, C. Gold, R. Brey, T. Gesell, P. Patton, M. Rudin, K. Eckerman, V. Rusetski, and S. Pagava entitled "Procedures and Quality Assurance for Calculating Dose Coefficients Using DCAL Software," *Health Phys.* (In Press).
- ♦ Journal article submitted by J. Shanahan, K. Eckerman, A. Arndt, C. Gold, P. Patton, M. Rudin, R. Brey, T. Gesell, V. Rusetski, S. Pagava entitled "Calculation of Dose Coefficients for Radionuclides Produced in a Spallation Neutron Source Utilizing NUBASE and the Evaluated Nuclear Structure Data File Databases," *Health Phys.* (In Press).



Schematic of DCAL System—adopted from ORNL/TM-2001/190 (Eckerman et al. 2001).

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Task 8

Development of a Systems Engineering Model of the Chemical Separations Process

Y. Chen, D.W. Pepper, and S. Hsieh

BACKGROUND

The chemical processing of used nuclear fuel is an integral component of any strategy for the transmutation of nuclear waste. Due to the large volume of material that must be handled in this first step of the transmutation process, the efficiency of the separations process is a key factor in the potential economic viability of transmutation strategies. The ability to optimize the chemical separation systems is vital to ensure the feasibility of the transmutation program.

Systems analysis, or total systems modeling, is one of the strongest tools available to researchers for understanding and optimizing complex systems such as chemical separations processes. Systems analyses permit researchers to present decision-makers concise evaluations of system options and their characteristic features. The primary goal of this project is to develop a systems model that can be used to parameterize and optimize chemical separations processes.

RESEARCH OBJECTIVES AND METHODS

This work includes reviewing and analyzing the AMUSE code structure, examining other possible implementations, defining software activities, developing a verification plan, and modifying and improving the software. This work also involves redefining the graphical user interface (GUI) to increase the utility of the AMUSE code suite as a stand-alone analytical package.

Developing a systems engineering model required discussions with Argonne National Laboratory personnel to identify pertinent

components of the chemical separations process. Each step required model development to establish its significance with regards to the overall process. Comprehensive model development involved defining the inputs and outputs from individual models and establishing how each connected to the other within in the chemical separations process.

RESEARCH ACCOMPLISHMENTS

This project developed software for a general-purpose systems engineering model named TRP System Engineering Model Program (TRPSEMPro) that will be used to improve productivity in the design process. The system model also includes various numerical optimization technologies and "Design of Experiments" study technologies.

Object-Oriented Analysis and Design was used for developing and implementing the TRPSEMPro system. A graphical notation, Unified Modeling Language, was employed to express object-oriented designs. Microsoft.Net architecture was used for system development and Visual Basic.NET was the major programming language behind the system. XML (Extensible Markup Language) was used widely to describe data and sets of elements and attributes that can be defined by researchers. XML Schema was used for describing the structure of the system engineering model. XML Database was used to store all the run-time data for the AMUSE module. Since significant experimental data will be generated and require systematic analysis, MS SQL Server 2000 database was selected for housing all run-time parameters and simulation results.

The model is combined with commercial software packages MATLAB OPTIMIZATION toolbox and SIMULINK module from Mathworks.

The system model, TRPSEMPro, considers input simulation modules from multiple disciplines with inconsistent input/output handles. The package with the aid of middleware can communicate with various simulation modules developed by other research groups and create an XML-based model description file. The critical components for the system engineering modeling include System Manager, Model Integration, Study Plan, and Solution Viewer.

The introduction of the middleware design provides flexibility

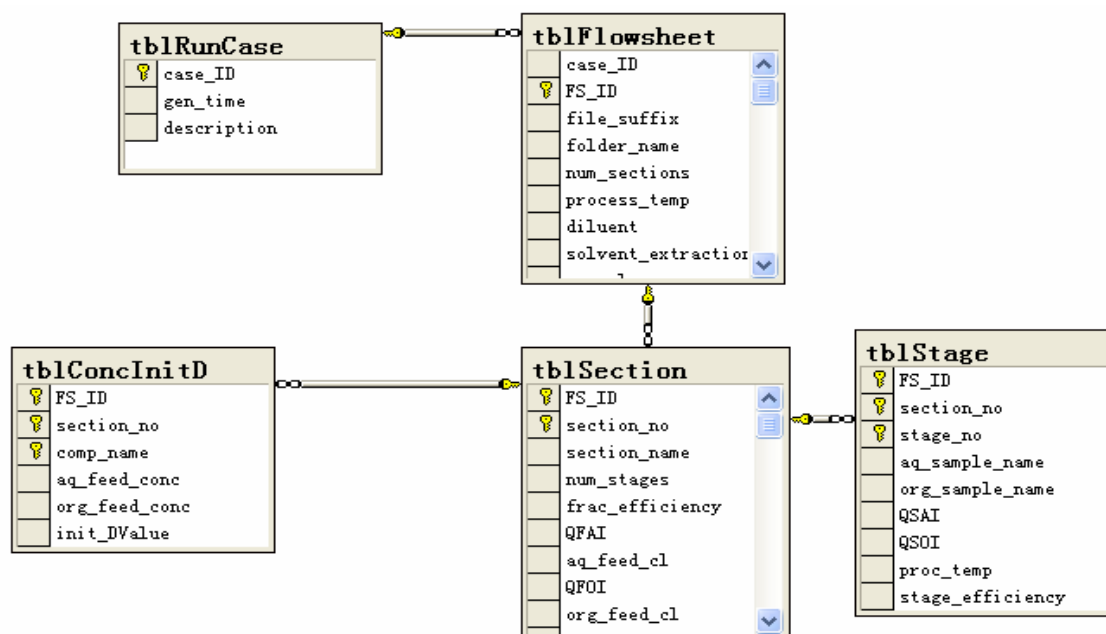


Diagram for the Structure of the Database Design.

to interface to other simulation modules without significant program modification. The demonstration code from AMUSE macros is kept intact during all system development stages. AMUSE-Simulator, is the middleware software package which was designed and implemented to serve as a bridge between the AMUSE code, and the systems engineering model, TRPSEMPPro. Such an approach can reduce the time-consuming modification on the system model side and keep flexibility on the simulation modules development side.

Further system enhancement allowed the user to select various process types. An interface for conducting multiple runs was created. The GUI included a list of variables, a range for those variables, all of which provide an envelope of end results.

TASK 8 PROFILE

Start Date: August 2001

Completion Date: August 2004

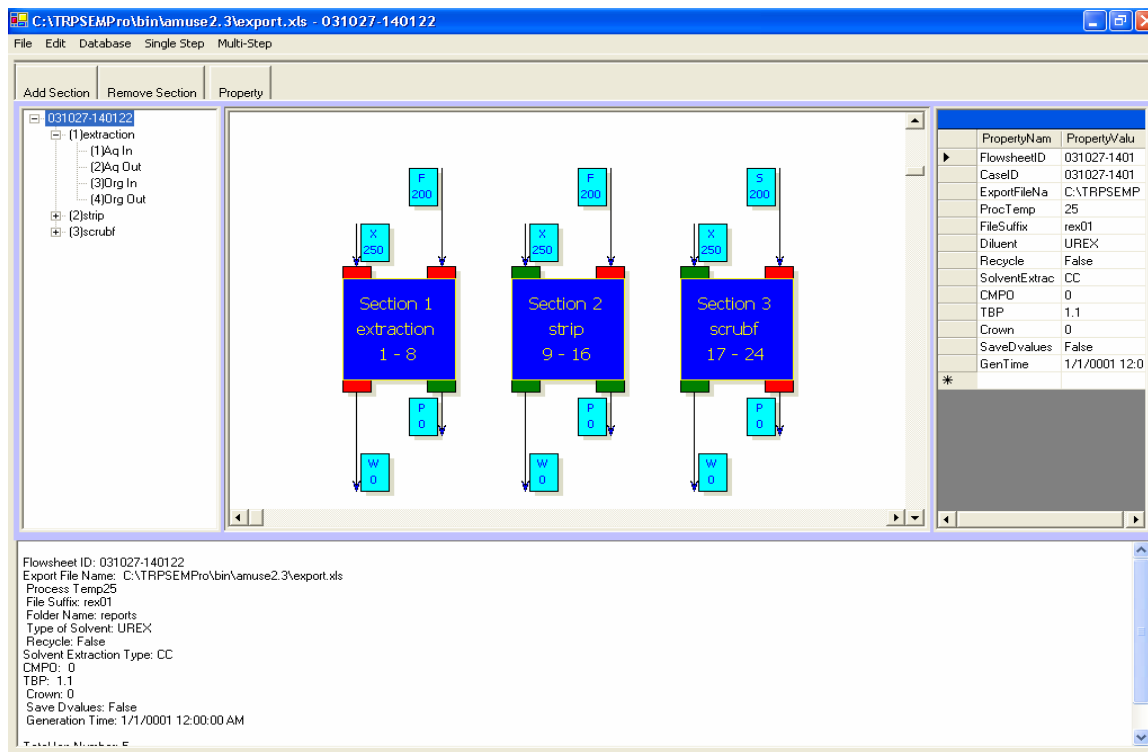
(This work is continued as Task 24, see pages 52-53.)

Thesis Generated:

Lijian Sun, M.S., Mechanical Engineering, "Development of a Systems Engineering Model for Chemical Separation Process," December 2003.

Conference Proceedings:

- "Development of Systems Engineering Model for Spent Fuel Extraction Process," IMECE 2004, International Mechanical Engineering Congress and Exposition Conference, Anaheim, CA, November 13-19, 2004.
- L. Sun, Royyuru, H., Hsieh, S., Chen, Y., Clarksean, R., Vandegrift, G., Copple, J., and Laidle, J., "Development of Systems Engineering Model for Spent Fuel Extraction Process," ICAPP-04, Pittsburgh, PA USA, June 13-17, 2004.
- H. Royyuru, Sun, L., Chen, Y., Hsieh, S., Clarksean, R., Pepper, D., Vandegrift, G., Copple, J., and Laidle, J., "Development of Systems Engineering Model For UREX Process," ASME International Mechanical Engineering Congress and Exposition, Washington, DC, November 16-21, 2003.
- H. Royyuru, Sun, L., Chen, Y., Hsieh, S., Clarksean, R., Pepper, D., Vandegrift, G., Copple, J., and Laidle, J., "Development of Systems Engineering Model For UREX Process," AccApp'03: Accelerator Applications in a Nuclear Renaissance, San Diego, CA, June 1-5, 2003.
- L. Sun, Chen, Y., Clarksean, R., and Laidler, J., "The Development of a Systems Engineering Model for the DOE Advanced Accelerator Applications Program," International Congress on Advanced Nuclear Power Plants, embedded topical meeting at the ANS Summer Meeting, Hollywood, Florida, June 9-13, 2002.



The main GUI for AMUSE-Simulator includes five parts as shown here. Menu and toolbar (Top Part) – where user can invoke all the available commands. Flowsheet contents displayed in tree view format (Left Part) – where user can select different section, stream. Flow-sheet contents displayed in way of drawing blocks (Middle Part) – where user can select different sections, streams by clicking mouse at corresponding area.

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Task 9

Design and Evaluation of Processes for Fuel Fabrication

G. Mauer

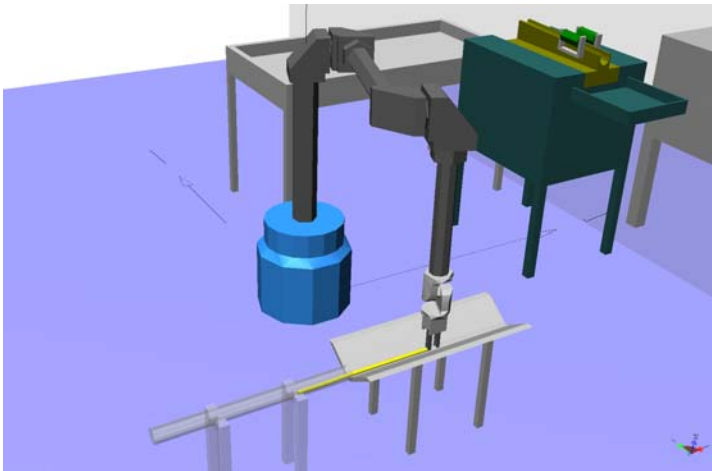
BACKGROUND

The safe and effective manufacturing of actinide-bearing fuels for any transmutation strategy requires that the entire manufacturing process be contained within a shielded hot cell environment. To ensure that the fabrication process is feasible, the entire process must be designed for remote operation. The equipment must be reliable enough to perform over several decades, and also easy to maintain or repair remotely. The facility must also be designed to facilitate its own decontamination and decommissioning. In addition to these design factors, the potential viability of any fuel fabrication process will also be impacted by a number of variables, such as the current state of technology, potential problem areas, deployment scaling, facility safety, and cost.

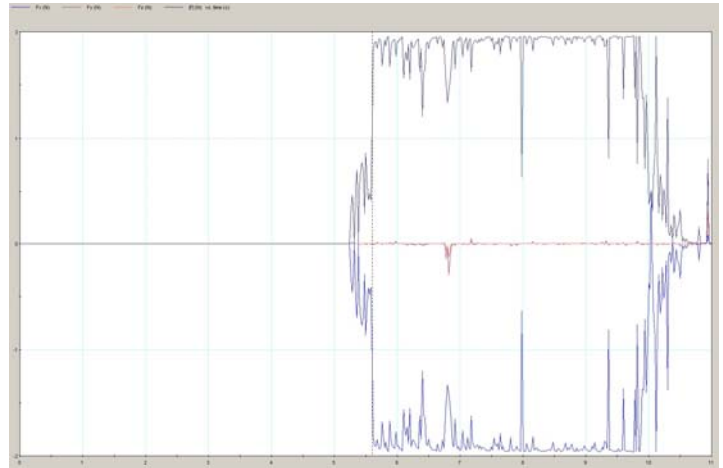
RESEARCH OBJECTIVES AND METHODS

The goal of this research project was to provide technical support to process designers working on the development of the fuel cycles for transmutation applications. Detailed process models were developed to better define the impact of fuel choice on the transmuter fuel cycle, including relative process losses, waste generation, and plant capital cost. These process models provide insight regarding required plant size and number of plants needed to mesh with the fuel recycling line. They also determine requirements for automation.

Manufacturing models for large-scale production in a hot cell environment were also developed. Combined, these two models allow the assessment of plant layout, and provide the framework for estimation of plant capital and operating cost estimates, and for feasibility in general. The need for development in the areas of robotic and sensor technology was assessed. The manufacturing technology developed for hot cell applications was also applicable to other, more general uses, where occupational hazards



The Waelischmiller robot inserts the fuel pins in the cladding tube.



Friction Force (N) between Second Pin and Cladding Tube vs. Time (sec) during Insertion.

prevent human presence near processes.

The research work was divided into several tasks and subtasks:

Methods and Processes – A literature survey and detailed analysis of the research and development pertaining to candidate processes for transmuter fuel manufacture was performed. Industry standards were used to refine equipment, instrumentation, and control specifications, and assessed the reliability and safety of operations.

Simulations – This task modeled manufacturing processes to generate a realistic assessment of plant layout, size, feasibility, and technology development required for large-scale remote fabrication of fuel. Modeling of the candidate fuel manufacturing processes was conducted using the MSC.visualNastran and ProEngineer simulation software tools. The modeling of powder-processed fuels was completed, and the modeling of other fuel types (metallic, TRISO etc.) was initiated.

Process and Equipment for Autonomous Manufacturing – This task developed an understanding of the cost and capability of current generation remotely operated equipment suitable for use in radiation environments. Monitoring of the market for equipment and components with regard to suitability for automated manufacturing under hot cell conditions was conducted.

Sensors, Controls, and Operational Safety – This task determined the adequacy of current technology and the need for suitable sensor technology development for deployment in hard radiation environments. A means to identify the precise location and spatial orientation of all parts in the robot's work envelope were implemented. The ability to position and handle materials along with trouble shooting techniques were evaluated. Radiation hardened vision systems appear to be promising technologies.

Cost, Feasibility, and Large Scale Deployment –

This task developed the database necessary to provide cost estimates and differential cost for various fuel manufacturing options. Efforts were initiated to tabulate and quantify estimates regarding projected cost, reliability, and plant life.

RESEARCH ACCOMPLISHMENTS

A special simulation model with a Waelischmiller hot cell robot was developed and coupled with MatLab control software. Matlab provides the interface with the robot and is used to control the system. This renders a realistic simulation of the forces and torques present during robot motion. A 3-D manufacturing process simulation using CAD models and the Newtonian dynamics of the moving components was developed.

Results exist in the form of movies, data sets, and images. Simulations for several robot types were developed and their proper kinematic configuration was verified. The simulations permit the detailed analysis of forces and torques in any modeled part or component.

While the simulation process generally worked flawlessly, the simulation time rose considerably as more details were added to the simulation. The speed of the simulation has been increased about 100-fold by moving to fast dual-processor computers.

Efforts to develop a vision-based methodology for locating and identifying objects within the robot's workspace were conducted using the Artificial Intelligence (AI) algorithm for object identification.

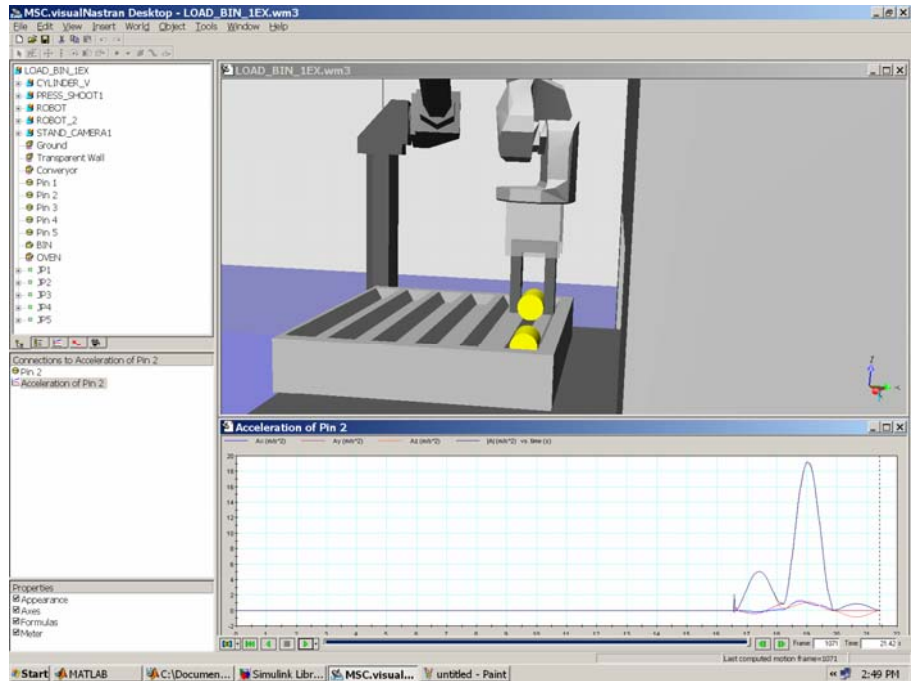
Another accomplishment involved the development of algorithms for knowledge based pattern recognition using IF (a set of conditions is satisfied) THEN (a set of consequences can be executed) routines. Other simulation variables established included pattern matching using clustered indexing vectors containing information about an object and feature vector indexing, where a 3-D object is segmented into a set of simple geometric features. Each feature is stored with its vector segmentation and geometry information (magnitude, inner angle, etc.).

TASK 9 PROFILE

Start Date: August 2001

Completion Date: August 2004

(This work is continued as Task 22, see pages 48-49.)



Visual Nastran Analysis of Pellet accelerations. The simulation verified that pellet's acceleration did not exceed a specified maximum of 20 m/s².

Thesis Generated:

Jae-Kyu Lee, Ph.D., Department of Mechanical Engineering, "Three Dimensional Pattern Recognition using Feature-based Indexing and Rule-based Search," December 2003.

Journal Article:

J.K. Lee and G. Mauer, "Feature-Based Pattern Recognition and Object Identification for Telerobotics," submitted to IEEE/ASME *Journal of Mechatronics* in August 2004 (under review).

Conference Proceedings:

G.F. Mauer and J. Renno, "Virtual Testing of Robotic Assembly Processes for Hot Cells," *Proceedings*, 10th International Conference on Robotics & Remote Systems for Hazardous Environments, March 2004.

G.F. Mauer and J. Renno, "Design and Analysis of Robotic Manufacturing Processes," *Proceedings*, American Nuclear Society Winter Annual Meeting, New Orleans, LA, November 2003.

G.F. Mauer, "Design and Evaluation of Processes for Transmuter Fuel Fabrication," *Proceedings*, American Nuclear Society Winter Annual Meeting, November 2002.

G.F. Mauer, "Object Recognition Over An Expanded Range Of Viewing Angles Using Indexing Methods," *Proceedings*, CAINE 2002 conference, San Diego, CA, November 2002.

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Task 10

Development of a Mechanistic Understanding of High-Temperature Deformation of Alloy EP-823

A. K. Roy and B.J. O'Toole

BACKGROUND

During the transmutation process, a significant amount of heat can be generated in a molten lead-bismuth-eutectic (LBE) target, which will be contained in a subsystem structural container made of a suitable martensitic iron-chromium-molybdenum (Fe-Cr-Mo) stainless steel such as Alloys EP-823, HT-9 and 422. These materials will be subjected to high tensile stresses while they are in contact with the molten LBE at temperatures ranging between 400 and 600°C. Therefore, a research program was conducted to evaluate the deformation characteristics of all three alloys in properly heat-treated conditions at temperatures relevant to the operating conditions.

RESEARCH OBJECTIVES AND METHODS

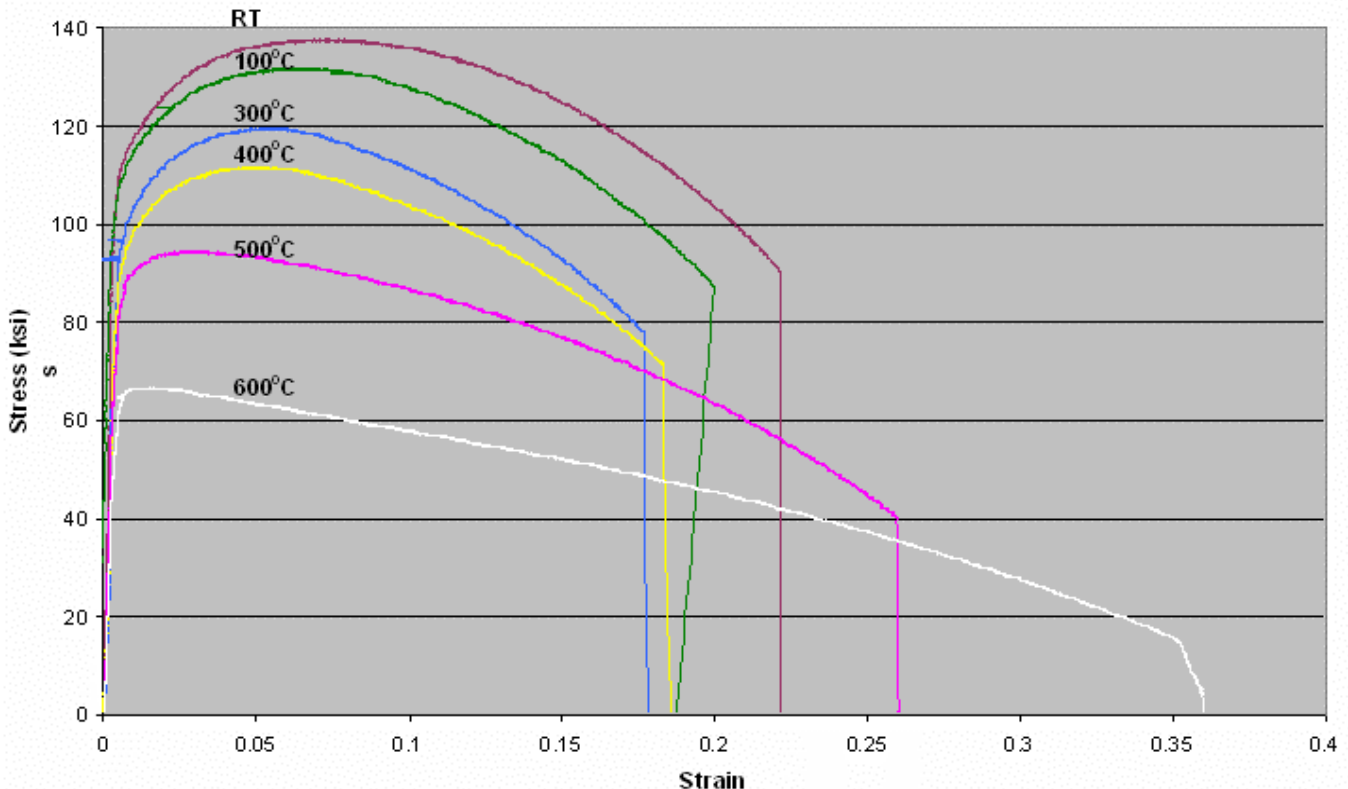
Experimental heats of Alloys EP-823, HT-9 and 422 were vacuum-induction-melted, followed by forging and hot rolling. The hot-rolled bars were subsequently thermally treated to produce a fully tempered and fine-grained martensitic microstructure without any retained austenite. They were austenitized at 1010°C, oil-quenched, and tempered at 621°C. The tempering operation was performed for 1.25, 1.75, and 2.25 hours, respectively, to study the effect of tempering time on the tensile properties. The hardness of all materials, before and after tempering, was measured

using the Rockwell hardness scale. The tensile properties were determined at temperatures ranging from ambient to 600°C using smooth cylindrical specimens at a strain rate of 10^{-3} sec^{-1} according to the ASTM Designation E 8. A minimum of two specimens was tested under each condition, with the average value recorded. The metallurgical microstructures of the tested specimens were evaluated by optical microscopy. The primary fracture surface of the tensile specimens was analyzed by scanning electron microscopy (SEM) to determine the extent and morphology of failure. The resultant data include the percentage elongation (%El), percentage reduction in area (%RA), yield strength (YS), and ultimate tensile strength (UTS) as functions of the testing temperature and thermal-treatments. At least two specimens per material were tested under each of the three metallurgical conditions at the desired temperatures.

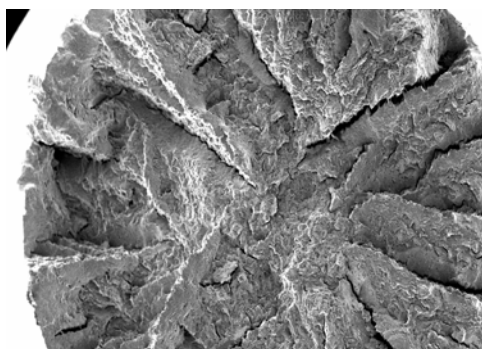
RESEARCH ACCOMPLISHMENTS

The significant conclusions drawn from this investigation are summarized below:

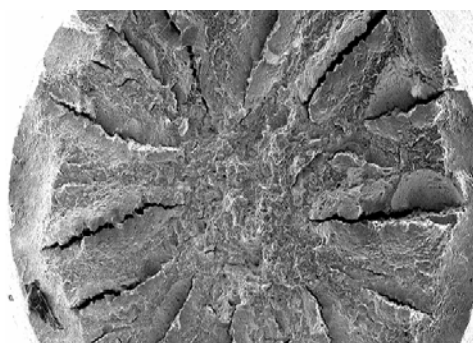
- The hardness of all three austenitized and quenched alloys was significantly reduced due to tempering, showing a gradual reduction with increasing tempering time.
- The magnitude of the yield, ultimate and failure stress was gradually reduced with increasing temperature, showing significant reductions at temperatures above 400°C.



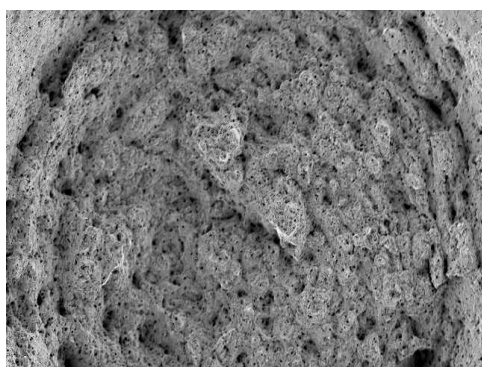
Stress-strain curves for Alloy HT-9 at different temperatures.



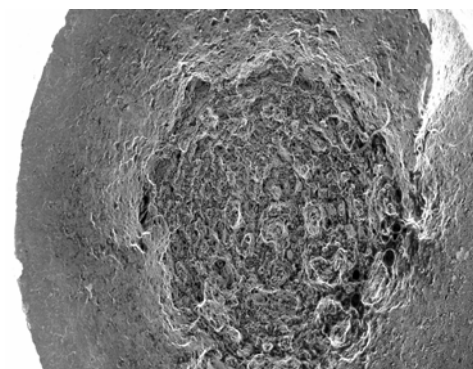
Room Temperature



100°C



300°C



600°C

Scanning Electron Microscope micrographs of Alloy HT-9 at various temperatures (35X).

- The extent of ductility in terms of %El and %RA was reduced to some extent in the temperature regime of ambient to 300°C due to strain hardening. However, beyond 300°C, the magnitude of these parameters was enhanced due to increased plastic flow.
- The morphology of failure was characterized by increased plastic deformation at elevated temperatures. Reduced cracking and dimpled microstructures were observed on the fracture surfaces indicating improved ductility at higher temperatures.
- The tempering time did not influence the metallurgical microstructure and the resultant tensile properties to any great extent irrespective of the testing temperature.

TASK 10 PROFILE

Start Date: August 2001

Completion Date: August 2004

Theses Generated:

Srinivasa R. Kukatla, M.S., Department of Mechanical Engineering, "Corrosion and High-Temperature Deformation Characteristics of a Target Structural Material for Transmutation Applications," June 2004.

Venkata Nagarjuna Potluri, M.S., Department of Mechanical En-

gineering, "Effect of Heat Treatment on Deformation and Corrosion Behavior of Type 422 Stainless Steel," August 2004.

Bhagath Yarlagadda, M.S., Department of Mechanical Engineering, "Elevated Temperature Mechanical Properties and Corrosion Characteristics Evaluation of Alloy HT-9," August 2004.

Journal Article:

A.K. Roy, S. R. Kukatla, B. Yarlagadda, V. N. Potluri, M. Lewis, M. Jones and B. J. O'Toole, "Tensile Properties of Martensitic Stainless Steels at Elevated Temperatures," *Journal of Materials Engineering and Performance*, ASM International, April 2005, Vol. 14, No. 2, pp. 212-218.

Conference Proceedings:

A.K. Roy, S.R. Kukatla, and B. Yarlagadda, "High Temperature Deformation Characteristics of Martensitic Stainless Steels," Society for the Advancement of Material and Process Engineering (SAMPE) International Technical Conference, Long Beach, CA, May 16-20, 2004.

S.R. Kujatla, V.N. Potluri, and B. Yarlagadda, "Temperature Effect on Mechanical Properties of Target Structural Materials," full technical paper, ANS Student Conference, Madison, WI, April 1-4, 2004.

M. Lewis, M. Jones, A.K. Roy, and B.J. O'Toole, "High-Temperature Deformation of Alloy EP-823 for Transmutation Applications," American Nuclear Society Conference, San Diego, CA, June 1-5, 2003.

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Brendan J. O'Toole, Associate Professor, Mechanical Engineering Department

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John Motaka, Undergraduate Student, Mechanical Engineering Department

Collaborator

Stuart A. Maloy, AFCI Materials Team Leader, Los Alamos National Laboratory

Task 11

Nuclear Criticality, Shielding, and Thermal Analyses of Separations Processes for the Transmutation Fuel Cycle

W. Culbreth and D. Beller

BACKGROUND

The first step in any transmutation strategy is the separation of radionuclides in used nuclear fuel. The current separation strategy supporting the Advanced Fuel Cycle Initiative (AFCI) program is based on the use of a solvent extraction separation process to separate the actinides, fission products, and uranium from used commercial nuclear fuel, and on the use of pyrochemical separation technologies to process used transmuter fuels. To separate the fission products and transuranic elements from the uranium in used fuel, the national program is developing a new solvent extraction process, the Uranium Extraction Plus, or UREX+, process based on the traditional solvent extraction reprocessing technologies.

Preparing fuel for possible burn up in light water reactors, fast reactors, or accelerator-driven systems involves various chemical processes to partition the transuranics (neptunium, americium, plutonium, and curium) from the fission products. This results in waste streams that are highly radioactive and require radiation shielding for safety. These transuranic elements pose varied criticality, thermal, and radiation risks during storage and handling. Additionally, the radioactive decay of strontium and cesium waste products of the UREX+ technique produce roughly half of the thermal products and gamma radiation emissions in spent fuel. These radioisotopes require storage for approximately 300 years before heat and radiation hazards decrease to a safe level.

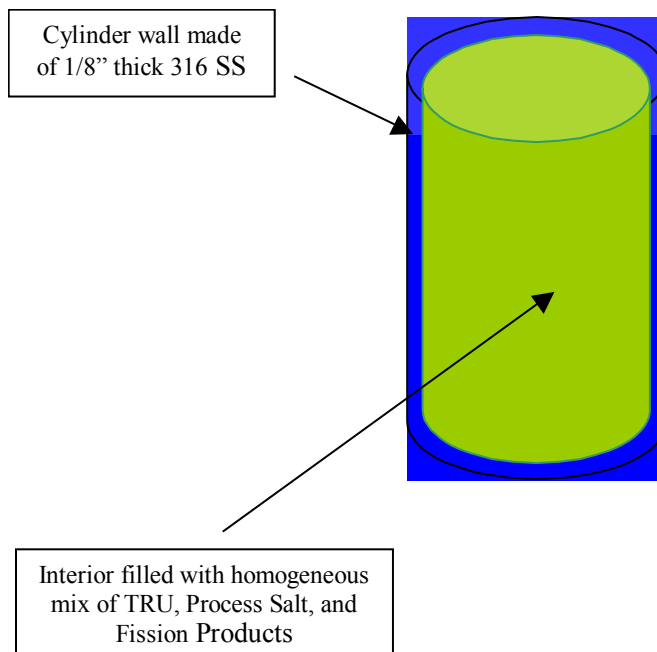
As the volume of waste requiring treatment increases, a higher probability exists that fissionable isotopes of plutonium, neptunium, and curium can accumulate and form a critical mass. Criticality concerns warrant an assessment of the effective neutron multiplication factor, or k_{eff} , to prevent a possible sustained fission reaction. Maintaining k_{eff} below a safe level (<0.95) prevents criticality events. This parameter can be computed for any combination of fuel and geometry using Monte Carlo neutron transport codes. Monte Carlo simulations establish the best means of examining the criticality safety of the proposed separation processes, and allow engineers to develop proper safety measures for the reprocessing and fabrication of actinide fuels.

Candidate storage containers also require analysis to assess the need for radiation shielding. Since minor actinides generate significant amounts of heat through radioactive decay, proposed containment measures must be designed to avoid excessive temperatures. Radioactive decay also generates heat that can lead to melting of the fuel during storage and handling.

RESEARCH OBJECTIVES AND METHODS

The primary goal of this research program was to provide the nuclear and thermal modeling support for the development of this new separation process. The assessments of nuclear criticality, radiation for shielding, and thermal analyses of wastes in the Cs/Sr, Pu/Np, and Cm/Am waste streams will assist in designing the UREX+ process. This project was identified as a critical R&D need of the Chemical Technology Division (CTD) at the Argonne National Laboratory (ANL) as safety concerns associated with criticality, shielding, and heat buildup must be addressed prior to further development of the UREX+ process.

UNLV students used nuclear analysis codes to perform assessments of k_{eff} at different points in the separation processes that have been identified by the project collaborators at ANL-CTD. They also worked on problems to assess the need for radiation shielding and to develop software to assess the possibility of excessive temperatures due to radioactive decay in separated wastes. ANL-CTD has provided sample fuel process geometries and compositions for calculation of k_{eff} as a function of the relative concentrations of process salt, transuranics, and fission products.



Cylindrical problem with TRU, process salt, and fission products.

RESEARCH ACCOMPLISHMENTS

An investigation and analysis of criticality and thermal effects for the safe storage of curium was completed. The assessment involved determining k_{eff} as a function of fuel burnup, initial enrichment, and time since irradiation. Additionally, since curium generates a substantial quantity of decay heat, an analysis was completed to determine the mass of curium that will lead to temperatures high enough to melt the metal. A spherical geometry was used in the analysis. Heat removal from the sphere was assumed to be a combination of natural convection and radiation heat transfer. This heat transfer analysis was also modified and resulted in an analysis that utilized a more sophisticated and suitable cylindrical container. A report developed for Dr. Laidler at ANL described the in-depth investigation regarding the criticality and thermal properties of curium. The heat transfer spreadsheet was used for other combinations of minor actinides as indicated by ANL.

Investigators also investigated the properties of the other minor actinides, including plutonium and americium. A study was conducted on the values of k_{eff} and ultimate temperature for varying combinations of plutonium, americium, and the remaining minor actinides.

UNLV students used nuclear analysis codes SCALE 4.4 and/or MCNPX to perform assessments of k_{eff} at different points in separation processes that have been identified by ANL-CTD. They also worked on problems to assess the needs for radiation

shielding and develop software to assess the possibility of excessive temperatures due to radioactive decay in separated wastes. ANL-CTD has provided sample fuel process geometry and composition for calculation of k_{eff} as a function of the relative concentrations of process salt, TRU actinides, and fission products. The research team analyzed the cesium/strontium waste stream, the plutonium/neptunium waste stream, and the americium/curium waste stream.

TASK 11 PROFILE

Start Date: August 2001

Completion Date: August 2004

Thesis Generated:

Srinivasa Elizabeth Bakker, M.S., Mechanical Engineering Department, "Criticality and Thermal Analysis of Separated Actinides in Transmutation," November 2003.

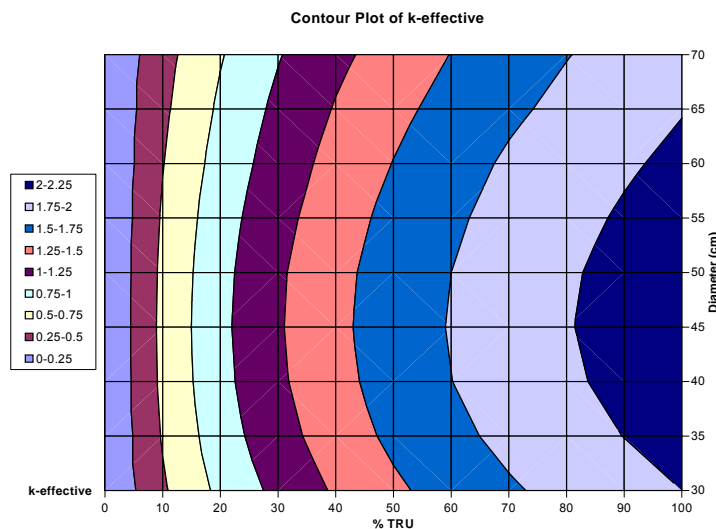
Reports:

B. Culbreth, E. Bakker, and J. Viggato, "The Fission Properties of Curium Separated from Spent Nuclear Fuel," Department of Mechanical Engineering, University of Nevada, Las Vegas, April 2002.

B. Culbreth, D. Lowe, and J. Viggato, "Assessment of Criticality Safety for Cylindrical Containers to be Used In the Processing of Spent Fuel," Department of Mechanical Engineering, University of Nevada, Las Vegas, October 28, 2001.

Cm Metal Cylinder		Criticality		Heat Transfer	
		rad (cm)	mass (kg)	rad (cm)	mass (kg)
	bare	4.6	82.52	1.1	1.129
	water	2.7	16.69	3.3	30.48
Cm ₂ O ₃ Cylinder		Criticality		Heat Transfer	
		rad (cm)	mass (kg)	rad (cm)	mass (kg)
	bare	5.4	125.59	1.55	2.74
	water	3	21.53	2.25	8.37
Am ₂ O ₃ Cylinder		Criticality		Heat Transfer	
		rad (cm)	mass (kg)	rad (cm)	mass (kg)
	bare	11.2	1032.28	1.6	3.01
	water	10.5	850.58	1.9	5.04
Am ₂ O ₃ +Cm ₂ O ₃ Cylinder		Criticality		Heat Transfer	
		rad (cm)	mass (kg)	rad (cm)	mass (kg)
	bare	10	737.9	1.4	2.02
	water	9.3	593.54	2	5.88

Recommendations for Cm and Am oxide inventories based on criticality and melting temperature.



Contour Plot of the Effective Neutron Multiplication Factor as a function of cylinder diameter and % TRU in the mixture.

Research Staff

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Denis Beller, Research Professor, Mechanical Engineering Department

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Collaborators

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Task 12

Radiation Transport Modeling using Parallel Computational Techniques

W. Culbreth and D. Beller

BACKGROUND

One of the most significant tools available for the design and analysis of accelerator-driven systems, such as the systems proposed for transmutation, is the high-energy particle transport code MCNPX. The MCNPX code suite, developed by the national laboratories, allows researchers and engineers to model the complex interactions of high-energy particles with the target and related systems, including the spallation reaction and subsequent neutron multiplication expected in the accelerator targets.

The next stage in the development of the MCNPX code suite is to validate the code by comparing the theoretical predictions from the models with experimental observations. Additionally, the nuclear database, particularly the cross sections (i.e., reaction probabilities) for high-energy particle interactions, needs to be revisited to reduce the uncertainties associated with key nuclear properties.

The Department of Energy, through its national laboratories, has initiated several experiments geared towards removing uncertainties in the MCNPX libraries, with more in the planning stages. These experiments utilize the proton and neutron beam lines at the LANSCE proton accelerator at the Los Alamos National Laboratory to irradiate a target, producing a pulse of neutrons which are observed by the experimenters. The results of these experiments are then compared against the predictions from the MCNPX models of the system. By comparing the predicted system behavior to the data acquired from the experiments, the experimenters will be able to validate the MCNPX code and its nuclear data libraries.

Through this project, UNLV researchers are involved in support of these experiments by developing the system models in MCNPX and benchmarking/validating the models against the experimental results. UNLV students have also been involved in conducting experiments at LANL and in assisting researchers in designing new experiments.

RESEARCH OBJECTIVES AND METHODS

The second year of this project involved modeling several aspects of the LANSCE beam experiments:

- Modeling targets of varying diameter in air, in a vacuum, and in the presence of humid air;
- Modeling various proton beam profiles;
- Modeling the effects of off-axis proton beam impingement on the target;
- Modeling the asymmetry introduced by the steel table below the target;
- Modeling the effect of varying ratios of Pb to Bi and the effect of impurities; and



Robert O'Brien (left of center) and Daniel Lowe (far right) are both undergraduate Mechanical Engineering students working on the project

- Modeling the system, including other structures within the test room.

With the experience gained through modeling these systems, the UNLV researchers plan, with the assistance of their national laboratory collaborators, to develop a benchmark program for the neutron leakage tests and other tests related to transmuter development. A comprehensive three-dimensional computer-aided design (CAD) image of the LANSCE experiments was prepared using ProEngineer to help benchmark the experiments and provide accurate geometric data for MCNPX modeling.

RESEARCH ACCOMPLISHMENTS

Undergraduate student Daniel Lowe worked on neutron spallation tests at the LANSCE facility (Summer 2002). He performed MCNPX runs and worked on calculations for initial benchmarking data. His early MCNPX calculations helped the experimenters determine where foil packets should go and what types of neutron flux to expect from these foils. He also prepared foils to determine neutron flux from the experiment and assisted in radiation counting of the foils. Mr. Lowe completed Solid Works CAD models of the Blue Room at LANSCE and conducted MCNPX simulations of the summer experiments when he returned back to UNLV. His MCNPX runs included estimations of the effect of the proton beam striking the target at positions slightly off of the centerline. He also estimated the neutron energy spectra expected from the time-of-flight neutron detectors.

Through MCNPX simulations of the neutron leakage from lead-bismuth targets, the UNLV team was able to assist in the design of the experimental configurations for the LANCSE experiments. These models were also used to predict the results for the experiments, and assist in positioning detectors for measuring the leaking. Similar computational support was also provided for proton activation experiments in sodium coolant.

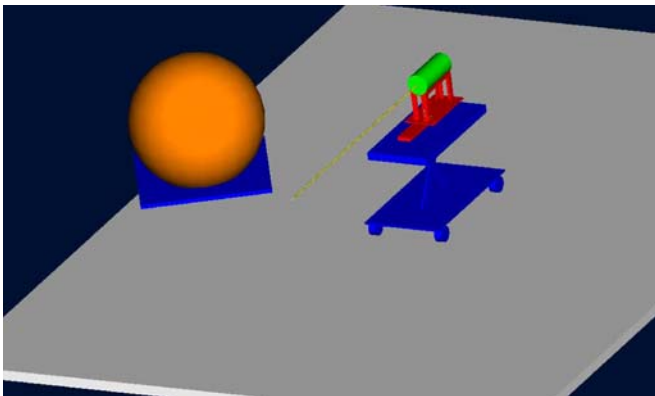
Extensive studies on how MCNPX performs with respect to MPI (Message Pass Interface) and PVM (Parallel Virtual Machine) have been run. PVM will no longer be supported by the LANL team after 2005, hence more emphasis is being put on how MCNPX runs with MPI on Beowulf system.

Parallelization of MCNPX for a Parallel Virtual Machine was completed. Message Passing Interface (MPI) bugs and compiling problems were resolved.

Analysis of linearization characteristics on a Beowulf cluster was completed. Work was then focused on characteristics of the Supercomputing Center and the linearization of criticality studies.

Benchmarking and optimization of MCNPX to run on multiple platforms was performed. This insured that the user will not be limited to a specific system type when running simulations. In addition, the MCNPX simulations of experiments was performed.

User guides were developed for future users. These will describe how to implement an optimized version of MCNPX on a heterogeneous cluster using a Message Passing Interface. Efforts to increase the speed of MCNPX on parallel clusters of computers was conducted and a preliminary graphical user interface (GUI) for MCNPX using open source code and tools was developed. The GUI interface is written in Visual Basic allowing easy inte-



Schematic of the experimental facility at LANSCE used for modeling.

gration into Excel codes that contain databases of results from criticality and heat transfer studies of waste storage containers.

With the help of Trevor Wilcox, a doctoral student in mechanical engineering, the MCNPX software was ported to a Beowulf cluster located in the Tiberti Laboratory at UNLV. The cluster has between 32 and 50 processors available to run a single MCNPX job.

TASK 11 PROFILE

Start Date: August 2001

Completion Date: August 2004

Thesis Generated:

Suresh B. Sadineni, M.S., Mechanical Engineering Department, "Benchmarking Photoneutron Production of MCNPX Simulations with Experimental Results," December 2002.

Conference Proceedings:

M.A. Reda, J.F. Harmon, and S.B. Sadineni, "Properties of Photoneutron Sources for Accelerator Driven Sub-Critical Systems," American Nuclear Society Conference, June 1-5, 2003, San Diego, CA.

M.R. James, R.T. Klann, G.L. Morgan, E.J. Pitcher, M.A. Paciotti, J.M. Oostens, J.E. Platte, and D.R. Lowe, "Measurements from Activation Foils of a Proton Irradiated Lead-Bismuth Target," American Nuclear Society Conference, June 1-5, 2003, San Diego, CA .



Experimental facility at LANSCE, Los Alamos, NM.

Research Staff

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Daniel Lowe and Robert O'Brien, Undergraduate Students, Mechanical Engineering Department

Collaborators

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Task 13

Developing a Sensing System for the Measurement of Oxygen Concentration in Liquid Pb-Bi Eutectic

Y. Jiang and B. Fu

BACKGROUND

Although liquid lead-bismuth eutectic (LBE) is a good candidate for the coolant that can be employed in a subcritical transmutation blanket, it is known to be very corrosive to stainless steel, the material used in the containment structure. To mitigate this problem, trace levels of oxygen can be introduced into the system, causing the formation of a protective oxide layer at the interface between the LBE and steel. The proper formation of this oxide layer largely depends on the accurate measurement and subsequent control of the oxygen concentration in liquid LBE.

Yttria Stabilized Zirconia (YSZ) oxygen sensors, using molten bismuth saturated with oxygen as the reference, have been utilized to accurately measure the concentration of oxygen dissolved in LBE. By measuring the voltage difference across the YSZ sensor, the oxygen concentration in test solutions can be determined relative to that in the reference solutions (the potentiometric method). The theoretical model for calculating oxygen concentration based on voltage measurements from YSZ sensors in static conditions is well understood. The real world performance of these systems, however, is less predictable.

For the past three years, calibration of YSZ oxygen sensors has been performed using both the experimental setup located in LANL and one apparatus designed by TRP Task 13 team members. A set of calibration curves (voltage vs. temperature, ranging from 300 to 500 °C, under various oxygen concentrations in liquid LBE) has been obtained. Different sensor references and signal wires have also been tested. Numerical simulation has been conducted to study the oxygen transfer in the calibration task.

RESEARCH OBJECTIVES AND METHODS

The research objectives of this project are as follows:

- To generate calibration curves of voltage versus oxygen concentration for the YSZ oxygen sensor system under various temperatures in liquid LBE.
- To determine the sensor characteristics of the YSZ sensor system.
- To determine oxygen dissolving rates in LBE under different temperatures in vitro.
- To study the effects of unwanted electrical conductivity, contributed by the mobility of the electrons at high temperatures, for more accurate oxygen measurement.
- To study alternative and promising oxygen measuring methods.

RESEARCH ACCOMPLISHMENTS

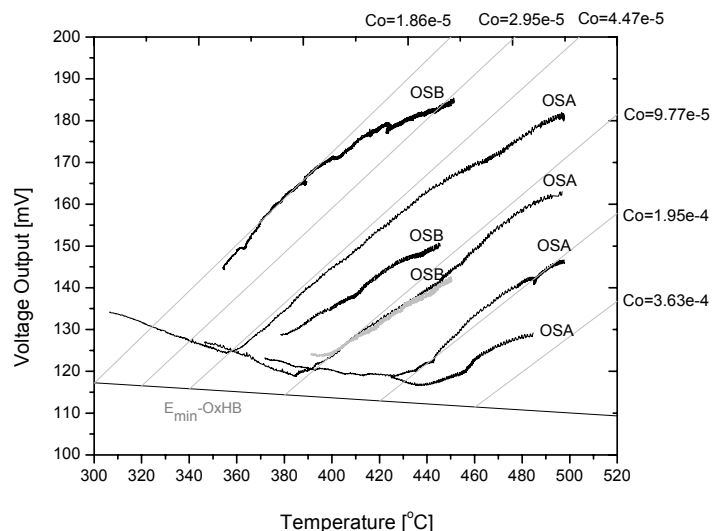
The first experimental setup consisted of a temperature controlled U-shape container, gas supplies and exhaust, a residual gas analyzer (RGA), a high-impedance electrometer, and a PC for data acquisition. The container is tightly sealed from outside atmos-

phere using a conflat flange except for gas inlet and outlet, and openings for insertion of thermocouple or RGA signal wire. Flexible heating tapes around the container can heat the liquid metal to the required temperature under the control of a temperature controller. The thermally insulated container was placed on a rocker to provide fluid motion that promotes mixing and homogenization of oxygen concentration in LBE.

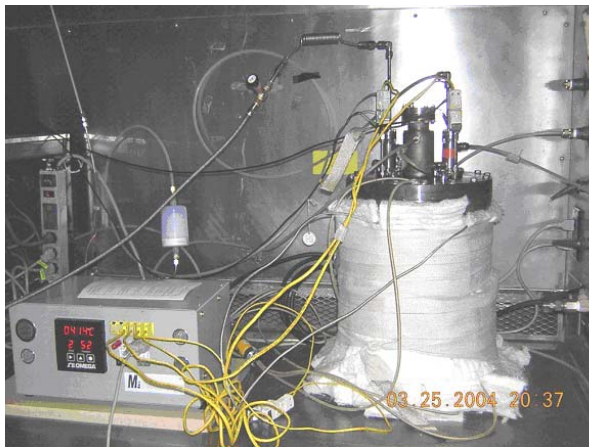
Although some calibration results were obtained using this setup, it had several shortcomings. For instance, it was impossible to heat the system to reach the desired high temperature (up to 750 °C). In addition, direct injection of the O₂/H₂ method adopted in this system is unlikely to produce a required extremely low oxygen level (ppm to tens of ppb) in liquid LBE. These problems in part were solved in another apparatus later developed by TRP Task 13 team members.

Calibration curves obtained from Oxygen Sensors A and B are shown in the figure below. It can be seen that after some initial transients, voltage-temperature curves first follow constant oxygen concentration lines according to the Nernst equation, and then turn to concentration saturation line.

- The slopes of experimental and theoretical curves are almost identical, ranging from 0.33 to 0.5. This indicates that the YSZ sensors are of high sensing quality;
- Being almost consistent with the theoretical results (a little above the theoretical calculation), the turning points clearly shown on the experimental curves for the sensor b indicate the regions at which the oxygen saturation occurs;
- Overlapping of the calibration curves for sensors A and B indicates the consistency in the sensors of the same design.



Sensor calibration results from two different sensors A & B.



Experimental apparatus developed at UNLV for the testing of the YSZ oxygen sensors.

FUTURE WORK

A number of practical problems have been encountered in this project including the contamination of the sensor chamber due to the leakage of liquid metal, and failure of the sensor due to the oxidization of the signal wire. These problems can become more serious when the sensor is used in a high temperature environment (up to 750 °C).

It has further been realized that for high temperature measurements, the main sources of oxygen measurement error result from the electronic contribution to the electrical conductivity of the electrolyte as well as the chemical reactivity between the electrolyte and electrode systems. As such, the reduction of the sensor's measurement errors can be achieved by proper selection of the solid electrolyte and the reference system.

Furthermore, a coating technology may be needed for better sealing of the sensors to operate in high temperature for prolonged hours.

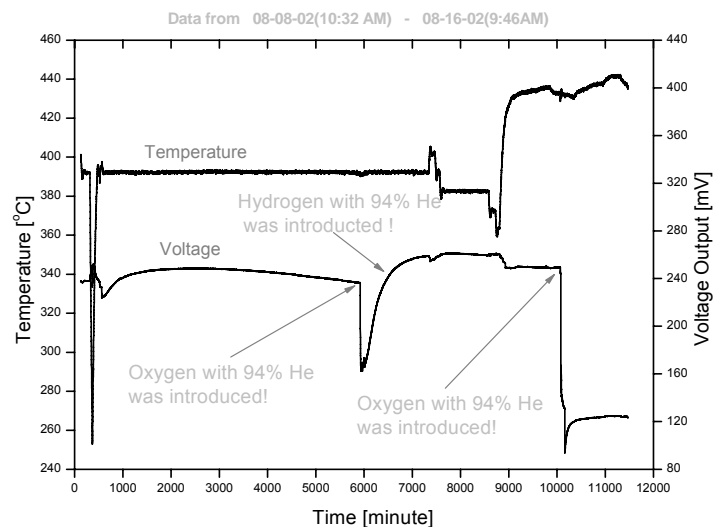
All of the above mentioned issues have to be considered to improve the YSZ sensors to operate in high temperatures. In addition, the improved high temperature sensors must be calibrated by intensive experimental work.

The future research work for this task shall include following components:

- 1) Try to mitigate the fluid that may leak into the sensor chamber.

ACADEMIC YEAR HIGHLIGHTS

- ◆ A manuscript entitled "Enhancement of Oxygen Transfer in Liquid Lead and Lead-Bismuth Eutectic by Natural Convection" was accepted for publication by *International Journal of Heat and Mass Transfer*.
- ◆ A paper entitled "Instrumentation of YSZ Oxygen Sensor Calibration in Liquid Lead-Bismuth Eutectic" was accepted by IEEE International Symposium of Circuits and Systems for the track Chemical Sensors, May 2005.



Response time to oxygen or hydrogen introduction using Sensor A.

- 2) Test different sensor signal wire materials and determine the best signal wire which can stand high temperature without oxidation.
- 3) Determine the protection of electrolyte of sensors at high temperatures.
- 4) Solve the assembly and sealing problems of sensors at high temperatures.
- 5) Fully test the new oxygen calibration apparatus and calibrate the new and improved sensors spanning the whole operational temperature range (350 °C to 750 °C), particularly, in temperature higher than 500 °C.
- 6) Develop silicon nitride and anodized alumina coating technologies for high temperature sensors.

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 Shahidur Rahman, Graduate Student, Department of Mechanical Engineering

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Ning Li, LBE Project Leader, and Wei Hang, Research Scientist, Los Alamos National Laboratory

Task 14

Use of Positron Annihilation Spectroscopy for Stress-Strain Measurements

A. K. Roy

BACKGROUND

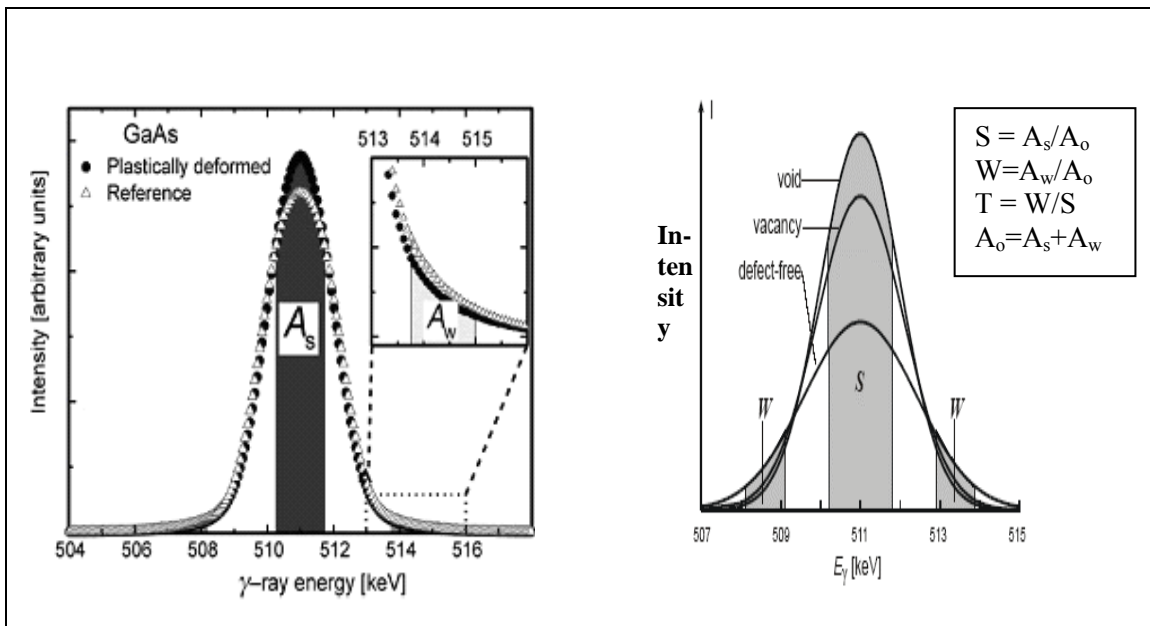
Engineering metals and alloys, when subjected to tensile loading beyond a limiting value, undergo plastic deformation resulting in lattice defects such as voids and dislocations. These imperfections interact with the crystal lattice, producing a higher state of internal stress, also known as residual stress, which can be associated with reduced ductility. Residual stresses are also generated in welded structures due to rapid solidification and resultant dissimilar metallurgical microstructures between the weld and the base metals. Development of these internal stresses is often influenced by incompatible permanent strain resulting from thermal and mechanical operations associated with welding and plastic deformation. These types of operations can cause premature failures in structural materials unless these stresses are relieved by thermal treatments, which are commonly known as stress-relief operations.

This project is focused on the evaluation of residual stresses in target structural materials by the state-of-the-art destructive and non-destructive techniques. In addition, microstructural evaluations have also been performed by metallographic techniques. More recently, the effect of post-weld-thermal-treatments (PWTT) on the internal stresses in welded specimens has been studied. Further, the characterization of defects by transmission electron microscopy (TEM) has been performed.

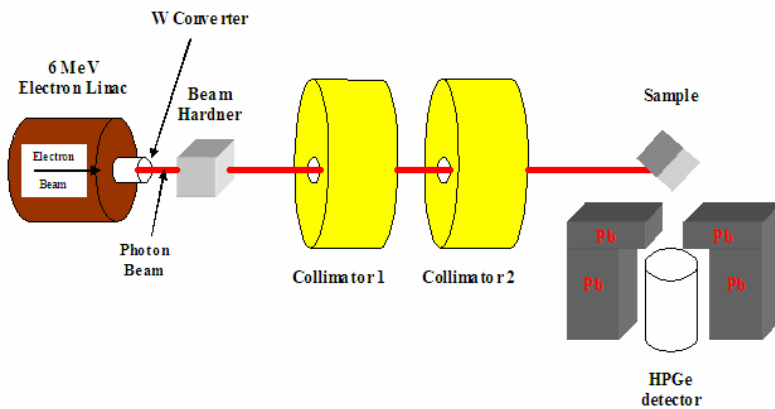
RESEARCH OBJECTIVES AND METHODS

The primary objective of this task is to evaluate the feasibility of the characterization of residual stresses in plastically-deformed and welded structural materials using a new nondestructive technique based on positron annihilation spectroscopy (PAS). The residual stresses measured by a modified PAS method have been compared to those measured by three other techniques namely, the ring-core (RC, destructive), X-ray diffraction (XRD, non-destructive), and neutron diffraction (ND, non-destructive).

All four techniques have been used to evaluate residual stresses in cold-worked, plastically deformed and welded specimens of austenitic Type 304L stainless steel (SS), and martensitic Alloys EP-823 and HT-9. Alloy EP-823 is a leading target structural material to contain the molten lead-bismuth-eutectic (LBE) nuclear coolant needed for fast spectrum operations of an accelerator-driven transmutation system (ADS). Type 304L SS is a universally-known corrosion resistant low-carbon iron-nickel-chrome alloy having optimum formability and weldability. Alloy HT-9 is known for its superior high temperature tensile properties. The metallurgical microstructures and the nature of defects have been analyzed by optical microscopy and TEM, respectively.



Characteristics of 511 KeV Gamma-Ray Energy Spectrum.



PAS Test Setup.

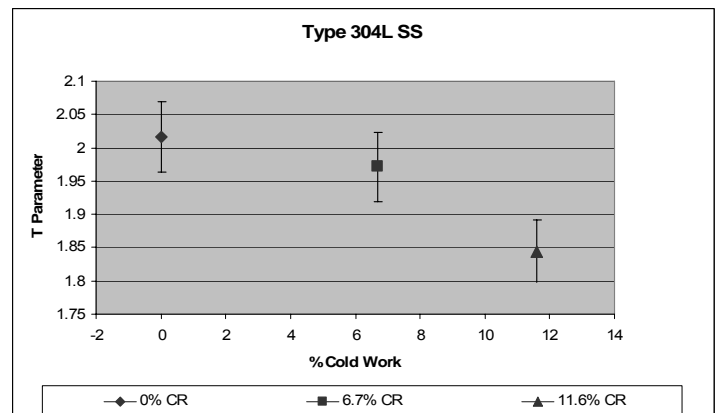
ACADEMIC YEAR HIGHLIGHTS

- ◆ Satish B. Dronavalli completed his M.S. thesis entitled "Residual Stress Measurements and Analysis by Destructive and Nondestructive Techniques," August 2004.
- ◆ Vikram Marthandam completed his M.S. thesis entitled "Metallurgical Characterization and Residual Stress Measurements of Target Structural Materials," August 2004.
- ◆ Anand Venkatesh completed his M.S. thesis entitled "Comparative Analyses of Residual Stresses in Target Sub-System Materials," August 2004.
- ◆ "Residual Stress Characterization in Structural Materials by Destructive and Nondestructive Techniques" was published in the *Journal of Materials Engineering and Performance*, ASM International, April 2005, Vol. 14, No. 2, pp. 203-211.
- ◆ "Residual Stress Measurements in Structural Materials by Non-destructive Technique" was presented at SAMPE 2005, Long Beach, CA, April 2005.

RESEARCH ACCOMPLISHMENTS

The significant results obtained to date are summarized as follows:

- The RC measurements on cold-worked (CW) specimens of Type 304L SS revealed tensile residual stresses, whereas compressive stresses were observed in Alloys EP-823 and HT-9 at a comparable cold-reduction (CR) level. This difference is attributed to different metallurgical characteristics of austenitic versus martensitic alloys.
- The PAS data were analyzed from the 511 keV energy spectrum in terms of three line-shape parameters S, W, and T. The S-parameter is sensitive to the annihilation with valence electrons and is defined as the ratio of the counts in the central region of the peak to the total counts in the peak. The W-parameter is more sensitive to the annihilation with high momentum core electrons and is defined as the ratio of the counts in the wings regions to the total counts in the peak. The T-parameter is simply the ratio of W to S. While the S parameter is directly proportional to the residual stress, the T parameter is inversely proportional to this stress. The PAS results indicate that, for Type 304L SS and Alloy EP-823, the T-parameter value was reduced with increased level of CR indicating higher residual stresses.
- The RC and ND data on welded specimens consisting of similar materials on both sides of the weld revealed tensile residual stresses adjacent to the fusion line. Reduced residual stresses were observed at locations away from the fusion line.
- The results of the PAS measurements on a welded specimen of Type 304L SS showed an enhanced S-parameter value near the fusion line indicating higher stresses.



T-Parameter vs Percent Cold Work.

- The ND measurements on the three-point-bent specimens showed compressive residual stresses at the convex surface and tensile stresses at locations close to the concave surface.
- The TEM micrographs revealed dislocations in Alloy EP-823, which was plastically deformed by CR.

FUTURE WORK

- Development of calibration curves for S and T parameters versus stress or strain.
- Characterization of residual stresses by the PAS and ND methods in welded specimens after PWTT.
- Characterization of defects by TEM.

Research Staff

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 Doug Wells, Ph.D., Associate Professor, Department of Physics, Idaho State University
 Farida Selim, Ph.D., Post Doctoral Researcher, Idaho Accelerator Center, Idaho State University

Task 15

Immobilization of Fission Iodine by Reaction with a Fullerene Containing Carbon Compound and Insoluble Natural Matrix

S.M. Steinberg, G.S. Cerefice, and D.W. Emerson

BACKGROUND

The recovery of iodine released during the processing of used nuclear fuel poses a significant challenge to the transmutation of nuclear waste. Iodine-129, a long-lived fission product formed by both commercial nuclear power generation and nuclear weapons production, is released when reprocessing nuclear fuel. Since iodine can be concentrated in the human thyroid, any uncontrolled release of iodine may result in an increased rate of thyroid cancer in the exposed population. For this reason, recovery of iodine is important for implementing any nuclear transmutation strategy.

The first step in any transmutation strategy is the processing of the used nuclear fuel. This step involves separating the used fuel into its constituent elemental components, allowing the recovery of the uranium, actinides, long-lived fission products, and other components, depending on the strategy and processes involved.

When used fuel rods are dissolved in concentrated nitric acid in preparation for actinide recovery, iodine is released from the fuel. A significant fraction of the iodine is lost to the vapor phase during this process, where it may potentially become a fugitive emission and be released from the plant. To avoid this, specialized filtration systems are used to try to trap and sequester the released iodine (and other fission product gases).

The primary goal of this research is to capture and immobilize the iodine released from these processes in a form that can easily be converted to a suitable target for neutron-induced transmutation. The investigators believe that iodine released during fuel reprocessing can be immobilized in a Fullerene Containing Carbon (FCC) compound or a Natural Organic Matter (NOM) matrix.

Natural organic matter (such as sphagnum moss, peat or brown coal) is an inexpensive and a renewable resource. Further processing of the trapped iodine using simple desorption or combustion processes should be able to produce iodine in a form suitable for transmutation. Furthermore, collaborators at the Khlopin Radium Institute (KRI) have proposed that the iodine-loaded FCC mate-

rial, when combined with ceramics, is stable enough for use as a long-term storage form, and may be usable as a transmuter target matrix.

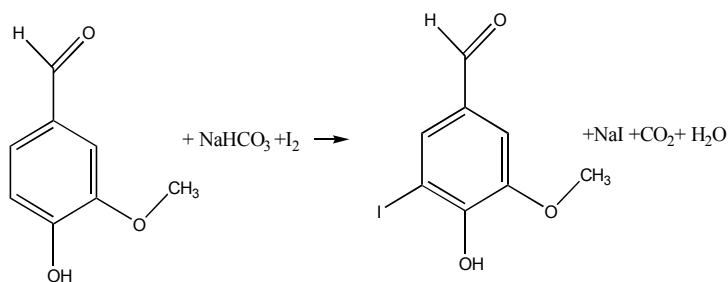
RESEARCH OBJECTIVES AND METHODS

The stability of the association of iodine with FCC and NOM products are studied. Product distributions for the various matrices under various reaction conditions were examined in order to maximize the binding of iodine. The recovery of the iodine from the sequestration matrices was also examined, along with the conversion of the iodine to matrices more suitable for geological storage and/or use as transmutation targets.

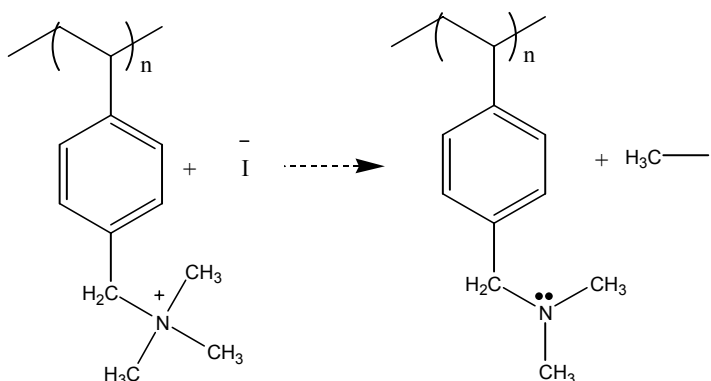
The following are the specific research objectives and goals:

- Develop bench-scale experimental set-up and procedures for simulating PUREX head-end vapor phase.
- Develop experimental procedures for evaluating iodine sequestering methods using bench-scale procedures.
- Develop FCC bearing material as potential iodine sequestration matrix.
- Determine binding of iodine to FCC and NOM.
- Examine alternate iodine sequestration matrices using techniques developed for FCC and NOM studies.
- Examine the effect of reaction conditions on binding.
- Elucidate the nature of the reaction products (volatile, hydrophobic, soluble, insoluble).
- Develop methodology and host matrix for converting sequestered iodine to solid matrix for evaluation as transmutation target and/or disposal matrix.
- Examine recovery of iodine from sequestration matrices.

The FCC compounds are developed and prepared by the KRI Research Industrial Enterprise (KIRSI). The KRI-KIRSI team research the impacts of process parameters on sorption of iodine, and examine the material properties, such as how iodine attaches to the FCC compounds. The KRI-KIRSI team also examines the



Ring addition of iodine to a phenolic compound. This reaction is an analogy for reaction with NOM.



Transformation of iodide to methyl iodide by pyrolysis of anion exchange resin.

conversion of the iodine loaded FCC compound to a stabilized matrix (similar to ceramic) for potential use as a disposal form, acceptable transportation material, or potential target material.

RESEARCH ACCOMPLISHMENTS

Highlights of accomplishments to date include the following:

- Fuel rod dissolution experiments were conducted and it was demonstrated that FCC and NOM can sequester iodine under these conditions.
- Nitrogen dioxide (NO_2) impact on iodine sequestration: Using the fuel rod simulator it was demonstrated that NO_2 (generated by metal dissolution in nitric acid) reduces iodine sorption for both FCC and NOM.
- Iodate Reduction studies: NOM was demonstrated to convert iodate to iodide and organoiodide at moderate pH. IOH was demonstrated to be an intermediate in the reduction process. Pyrolysis of NOM demonstrated that a large fraction of the iodate is converted to organoiodine.
- Efforts were continued to prepare methyl pyridinium resin. Methods were developed to prepare larger quantities of the methyl pyridinium resin in the chloride form. Recovery studies will be initiated.
- A preparative pyrolysis method was developed for forming methyl iodide. This technique will be used to recover sodium iodide. Using the preparative method, increased



Iodine System

ACADEMIC YEAR HIGHLIGHTS

- ♦ “Immobilization of Fission Iodine by Reaction with Insoluble Natural Organic Matter” by G.T. Schmett, G.M. Kimble, S.M. Steinberg, D.W. Emerson and G.S. Cerefice, was published in the Proceedings of the Actinide and Fission Product Partitioning & Transmutation, Eighth Information Exchange Meeting, OCED/NEA, Las Vegas, Nevada, November 9-11, 2004.
- ♦ “Abiotic Reaction of Iodine and Iodate with Sphagnum Peat” by S.M. Steinberg, G. Kimble, G.T. Schmett, and D.W. Emerson was presented as an extended abstract and poster at the American Chemical Society, Division of Environmental Chemistry (Volume 4, No. 1 - Spring 2005).

methyl iodide during pyrolysis was demonstrated as a function of reaction time reaction time for the case of the iodate-peat reaction.

- The reaction rate of iodine (as triiodide) was quantified in aqueous solutions. Using model compounds, it was demonstrated (as previously proposed) that the reaction is first order in the phenol and in I_3^- . The effects of temperature and pH on the reaction kinetics were measured. Iodine reaction measurements were made on a soluble alkali lignin a commercial humic acid and several model organics (vanillin, vanillic acid, syringic acid, p-hydroxy benzoic acid, and coumaric acid).

FUTURE WORK

Trials with NOM will be continued in the third year of the project. Additional sequestration experiments with the fuel rod simulator will be performed. Investigation into the speciation of iodine in the NOM in an exposed trap will be continued. Additionally, rate constants for the formation of iodate and for the formation of iodophenols will be estimated. The effect of pH on the reaction of iodine with NOM will continue to be investigated. Conversion of trapped iodide (via methyl iodide) to potential target materials will be studied and a bench scale method will be developed.

Research Staff

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Task 16

Evaluation of Fluorapatite as a Waste-Form Material

D.W. Lindle, O. Hemmers and D.L. Perry

BACKGROUND

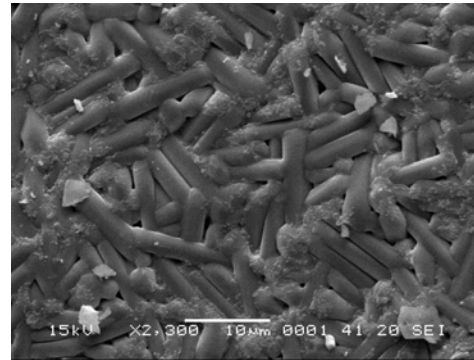
High Temperature Gas-Cooled Reactor (HTGR) systems are currently being designed and evaluated as part of the Advanced Fuel Cycle Initiative, both as a future nuclear reactor type (in the Generation IV reactor program) and as a potential system for burning plutonium in a dual-tier transmutation strategy. HTGR designs use a TRISO-coated fuel (a silicon-carbide and pyrocarbon composite coating) to provide much of the passive containment for radionuclides.

Although this fuel form is quite stable and comprises one of the key components in the safety performance of these reactor systems, TRISO-coated fuel is comparatively difficult to recycle. If HTGR systems are to be used as part of either the first tier of a transmutation strategy or as primary power reactors, the plutonium and other actinides in the used TRISO fuel must be processed to recycle plutonium and permit recovery of minor actinides and other fission products produced.

Argonne National Laboratory has proposed a new extraction procedure to handle TRISO-coated fuels, the Fluoride Extraction Process, or FLEX. The FLEX process is designed to separate the uranium in the fuel from the actinides and most fission products by taking advantage of the unique properties of uranium hexafluoride (UF_6). In the FLEX process, the used TRISO fuel is reacted with zirconium fluoride salt, forming UF_6 and the fluoride salts of the actinides and fission products. At process temperatures, the UF_6 volatilizes into a gas, and is released from the molten salt mixture. This leaves behind the actinides and most fission products in a fluoride salt, which is subsequently processed using pyrochemical techniques to recover the actinides and other long-lived fission products for transmutation. The UF_6 is then cooled, causing it to sublime into solid form, which is then further processed for disposal or reuse.

The primary waste stream from the FLEX process is the fission products from the fuel, which are in a zirconium fluoride salt at the end of the process. Due to the fluorine in this waste stream, the fluoride salts are unsuitable for conversion into the traditional borosilicate waste glass. Therefore, without a suitable disposal form, this process can not be deployed.

This research attempts to develop a waste form for disposing of the zirconium fluoride fission product waste stream. Fluorapatite, a naturally-occurring fluorinated calcium phosphate, has been identified as a potential matrix for the entombment of this waste stream. If the efficacy of fluorapatite-based waste-storage can be demonstrated, then new and potentially more efficient options for handling and separating high-level wastes, based on fluoride-salt extraction, will become feasible.



SEM micrograph of Ca_4SrFap (annealed sample)

RESEARCH OBJECTIVES AND METHODS

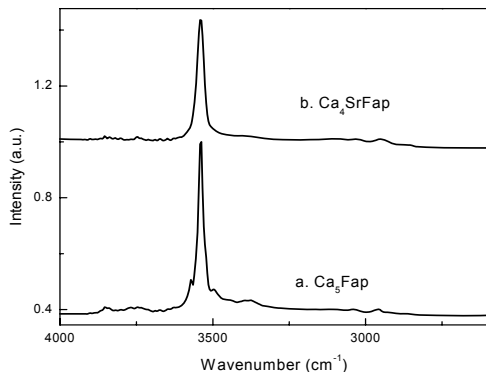
The following are the specific research objectives:

- To develop a waste matrix for the disposal of the fission product waste stream from the FLEX process;
- To develop a process to make synthetic fluorapatite that incorporates the FP-bearing ZrF_4 salt;
- To develop a fundamental understanding of the chemistry of this new waste form in order to better predict its long term behavior in a repository environment;
- To develop a fundamental understanding of natural, fluoride-bearing mineral phases to use as natural analogs to bound the predicted behavior of the FLEX fission product waste stream.

Originally, the research effort had been divided along two parallel paths: the *Fabrication Path*, led by collaborators at the Khlopin Radium Institute (KRI) in St. Petersburg, Russia; and the *Characterization Path*, led by researchers from UNLV.

The Fabrication Path is focused on examining and evaluating various techniques for fabricating synthetic fluorapatite; synthesizing synthetic fluorapatite; and examining the impacts of waste loading and other fabrication process factors on the performance of the synthetic fluorapatite as a potential waste form.

The Characterization Path is focused on adapting and refining the X-ray spectroscopy techniques currently used to characterize borosilicate glass for use in examining the fluorapatite system. This path also encompassed the examination of the ceramic and synthetic mineral waste forms created at KRI, with subsequent examination of these techniques to develop a molecular-level understanding of natural fluorapatite and other fluorine-bearing natural phases as natural analogs for the waste form. These techniques will also be used to examine the changes in surface chemistry caused by environmental degradation of these materials.



IR spectra of Ca_5Fap and Ca_4SrFap after annealing.

Waste form development at KRI involves the formulation, synthesis, and examination of ceramic samples to investigate the impact of processing parameters and composition on material properties (e.g. homogeneity) and performance (via leach testing). The most promising fabrication process developed will be used to synthesize the ceramic in varying compositions to examine the impact of process parameters, ceramic formulation, and waste loading on the final ceramic phase. Based on these experiments, a baseline composition and fabrication process will be established. Finally, alternate fabrication processes, compositions, and potential alternate waste matrices will be examined and compared against the baseline composition.

Waste form characterization carried out at UNLV employs state of the art techniques that characterize the molecular structure of both natural fluorapatite and fluoride-bearing minerals and the fluorapatite-based ceramic waste form. Changes in the surface/interfacial chemistry of these materials as they undergo reactions with species in the environment will also be examined to help develop a basis for understanding the corrosion chemistry that the waste form and its natural analogs may experience under repository conditions. The UNLV researchers also synthesized several surrogate samples with help of the KRI collaborators in order to study their properties.

RESEARCH ACCOMPLISHMENTS

Research highlights for the third year can be summarized as follows:

- Applying x-ray spectroscopy and more-conventional characterization techniques (e.g., Fourier Transform Infrared Spectroscopy, SEM, XRD, Raman Spectroscopy) to synthesized samples of apatite and fluorapatite doped with

ACADEMIC YEAR HIGHLIGHTS

- G. Silva presented a paper “Characterization of the Thermal Stability of Zinc Containing Fluorapatite” at the American Nuclear Society Student Conference, Columbus, OH, April 14-16, 2005.
- C. Rodrigo presented a paper “Characterization of Fluorapatite as a Waste Form Material” at the American Nuclear Society Student Conference, Columbus, OH, April 14-16, 2005.

surrogates and compared those with baseline measurements of “pure” materials.

- Chemically prepared several samples in which some of the calcium in apatite materials is substituted by non radioactive actinide surrogates (Zn, Sr, Yt, Cs, Cu, Ni, Zr) or elements produced by decay of actinides.
- Chemically prepared apatite samples containing different Ca:Surrogate weight ratios and studying the physical properties of these apatites with different calcium to phosphorous molar ratios.
- Studied metal-containing apatites and fluorapatites with the same cadre of characterization techniques noted above to assess the degree of incorporation and any changes in the physical and chemical structure of the materials.

FUTURE WORK

The work is completing its third and final year of the project with the two graduate students finishing their Masters degree. The Characterization Path, led by the UNLV team, has been performing baseline spectroscopic studies of natural and pristine (no artificially added impurities) apatite materials as well as of surrogate loaded samples. The studies found that it is possible to load surrogates successfully into apatites and that it is important to control the by-products such as metal phosphates and metal fluorites that weaken and/or destroying the crystal structure. The amounts of surrogates that can be loaded strongly depend on the type of surrogate and these amounts still need to be determined. The ultimate goal is to use these techniques to achieve a molecular-level understanding of fluorapatite and other fluorine-bearing phases as natural analogs for waste-form materials. These techniques will also be used to examine changes in surface chemistry caused by environmental degradation.

Research Staff

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Task 17

Interaction between Metal Fission Products and TRISO Coating Materials

C. Heske

BACKGROUND

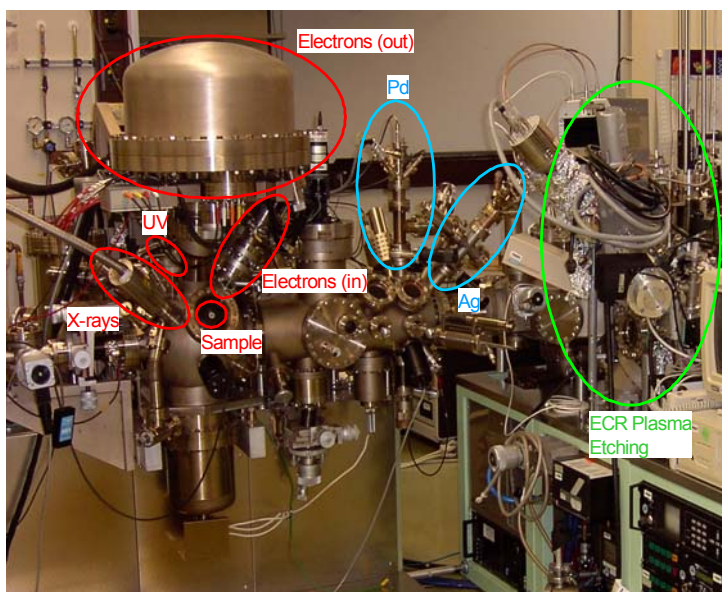
The goal of this project is to elucidate the chemical bonding and interface formation of metal fission products with the coating materials used in state-of-the-art TRISO fuel particles. Particular emphasis is placed on an analysis of intermediate chemical phases at the interface, the intermixing/diffusion behavior, and the electronic interface structure as a function of material choice (metal and coating materials), temperature, and external stress. Furthermore, the chemical state of some of the metal fission products will be assessed.

This project studies the interface formation of Pd, Ag, and Cs with SiC and pyrolytic carbon. Using the TRISO coating materials (and single crystal references) as substrates, interfaces will be prepared under controlled conditions in an ultra-high vacuum environment and will be studied with a variety of different spectroscopic and (when applicable) structural methods. In addition, realistic microstructures will be studied.

RESEARCH OBJECTIVES AND METHODS

The research objectives of this project are as follows:

- To give valuable information about failure mechanisms of TRISO particles and fission product transport.
- To give, through simulating experiments, indications for optimized irradiation testing and post-irradiation examinations within the AFCI effort at ORNL.
- To derive strategies to tailor the interface properties for an optimization of TRISO particles in terms of, e.g., chemical and long-term stability.



Picture of the four-chamber ultra-high vacuum apparatus. Red: surface spectroscopy; blue: metal deposition, green: surface modification.

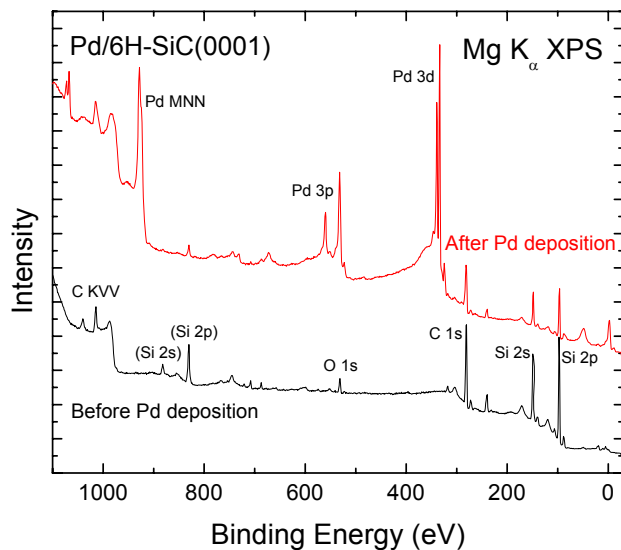
The combination of surface sensitive techniques (e.g., photoelectron spectroscopy) with bulk sensitive methods (e.g., X-ray emission spectroscopy) will probe the chemical properties as well as the diffusion behavior in several complementary ways. In addition, spatially resolving methods will be employed to characterize cross sectional profiles. A variety of surface modification methods will be applied ex-situ (e.g., for stressed coating layers) or in-situ (e.g., by ion bombardment) prior to or after the interface formation to study the dependence of the interface properties on the surface/interface morphology and quality of the coating material.

RESEARCH ACCOMPLISHMENTS

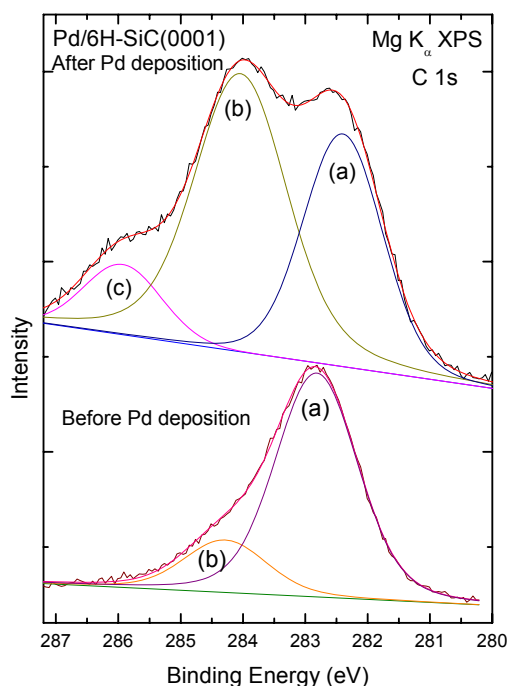
The project utilizes a four-chamber ultra-high vacuum surface science instrument (shown in the figure below, left), which combines several experimental techniques, including X-ray and UV photoelectron spectroscopy (XPS and UPS), X-ray and small-spot-electron-excited Auger spectroscopy (XAES and AES), low-energy electron diffraction (LEED), and in-situ ellipsometry. It allows the modification of surfaces by ion bombardment, plasma etching, annealing, and metal evaporation under strictly controlled conditions. The instrument was shipped from the University of Würzburg, Germany, in September of 2004 and arrived on campus in November 2004. After successful reassembly, all components are fully operational, and first calibration and surface science experiments are currently under way. Before dismantling the system for shipment at the University of Würzburg, first investigations of the Pd/SiC interface formation were conducted in Würzburg during the summer of 2004.

A second line of experiments is being conducted at the Advanced Light Source, Lawrence Berkeley National Laboratory (Beamline 8.0, SXF endstation). The first experimental campaign, in which the Pd/SiC interface was studied by soft X-ray emission spectroscopy and X-ray absorption spectroscopy, was conducted at the end of November 2004.

Several experimental runs were conducted to optimize the surface cleaning procedures for commercial SiC(0001) single crystal substrates. The figure on the next page (top, left) shows an XPS survey spectrum taken after a series of ion-sputter/annealing cycles to remove surface contaminants from the surface polishing process and the air exposure (in particular Ca, O, and water). As can be seen, only a small residual signal of oxygen is present, while all other prominent peaks are associated with the SiC bulk material. This surface was used to collect first data on the room temperature Pd/SiC interface formation by depositing a thin (less than 1 nm) layer of Pd (top spectrum in the figure). This leads to the observation of Pd-related lines and an attenuation of the SiC peaks. The Pd/SiC interface, a detailed analysis of the individual XPS peaks has been conducted. As an example, the figure (bottom, left) shows a close-up of the Carbon 1s peak.



X-ray photoelectron survey spectrum of a SiC(0001) single crystal before (bottom, black) and after (top, red) Pd deposition.



X-ray photoelectron spectra of the C 1s peaks before (bottom) and after (top) Pd deposition.

ACADEMIC YEAR HIGHLIGHTS

- ◆ Research on interactions between metal fission products and TRISO coating materials,” by C. Heske, G. Gajjala, and V. Marepally, was presented at the semi-annual meeting of the AFCE, Salt Lake City, UT, September 2004.
- ◆ “Interaction between metal fission products and TRISO coating materials (SiC),” by G. Gajjala, V. Marepally, T. Hofmann, J. White, C. Heske, L. Weinhardt, S. Hansen, O. Fuchs, and E. Umbach, was presented at the 49th Annual Meeting of the Arizona-Nevada Academy of Sciences, UNLV, April 9, 2005.
- ◆ “Interaction between metal fission products and TRISO coating materials (SiC),” by G. Gajjala, V. Marepally, T. Hofmann, J. White, C. Heske, L. Weinhardt, S. Hansen, O. Fuchs, and E. Umbach, was presented at the ANS Student Conference, Ohio State University, April 16, 2005.

Again, the bottom spectrum pertains to the clean SiC surface, while the upper spectrum was derived from the carbon atoms at and near the Pd/SiC interface. As indicated by the detailed peak-fitting analysis, it is evident that a bulk (a) and a surface (b) carbon component exist at the SiC surface. Upon deposition of Pd, a third species (c) is observed, which is tentatively interpreted as an interdiffusion-related carbon species. Furthermore, a strong interface species (b), a weakened bulk species (a), and a general upward shift of all electronic levels is observed. In an initial-state picture, the fact that the new species appear at higher binding energies indicates a charge transfer away from the carbon atoms. This finding is corroborated by the Si $L_{2,3}$ X-ray emission spectra (not shown) in which increased spectral weight was observed above the valence band maximum, i.e., near the Fermi energy, and interpret this as a Pd-induced transfer of partial charge to the Si atoms.

FUTURE WORK

Several parallel experimental paths will be followed in the upcoming project year. First, the study of the Pd/SiC interface will be continued to reproduce initial results (in particular the finding of two interface-related C species) and to investigate their dependence on external parameters, such as deposition temperature, Pd flux and thickness, and, in particular, substrate morphology. In the latter case, SiC films from the TRISO coating process will be investigated, as well as utilize suitable surface modification techniques (plasma etching, ion bombardment, etc.) to modify the interface properties.

Research Staff

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Task 18

Fundamental and Applied Experimental Investigations of Corrosion of Steel by LBE under Controlled Conditions: Kinetics, Chemistry Morphology, and Surface Preparation

J.W. Farley, A. L. Johnson, and D.L. Perry

BACKGROUND

This effort is a continuation of the work of Task 3 (see page 10), and the same overview applies. Advanced nuclear processes such as the transmutation of nuclear waste, fast reactors, and spallation neutron sources require advanced materials systems to contain them. In particular, a successful program in nuclear waste processing that includes transmutation in accelerator-driven systems and fast reactors requires structural materials that are stable in the presence of non-moderating coolants. A prime candidate for such a coolant is Lead Bismuth Eutectic (LBE).

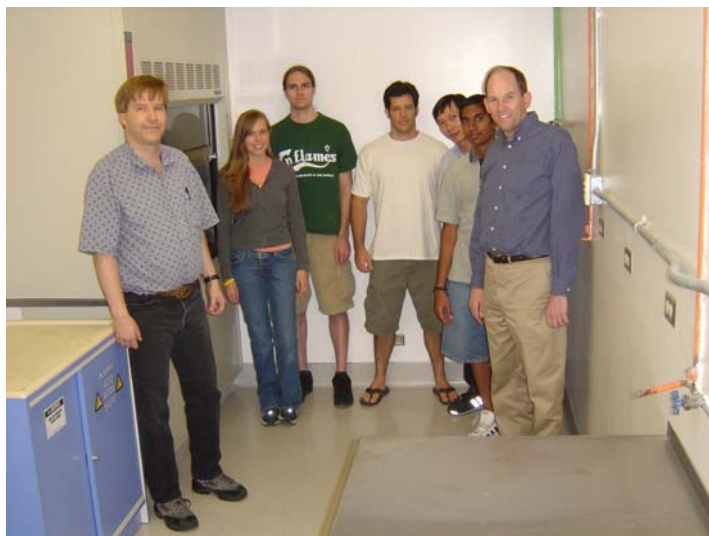
Materials in these systems must be able to tolerate high neutron fluxes, high temperatures, and chemical corrosion. For LBE systems, there is an additional challenge because the corrosive behaviors of materials in lead bismuth are not well understood. Most of the available information on LBE systems has come from the Russians, who have over 80 reactor-years experience with LBE coolant in their Alpha-class submarine reactors. The Russians found that the presence of small amounts of oxygen in the LBE significantly reduced corrosion. However, a fundamental understanding and verification of oxygen's role in the corrosion of steels is incomplete.

RESEARCH OBJECTIVES AND METHODS

Previously, various steel samples that were exposed to lead bismuth eutectic were analyzed as part of the national program to develop LBE and allied technologies under TRP Task 3. In particular it was found that cold rolled 316L and a silicon modified HT9-like alloy EP823 had particularly low corrosion rates. The 316 systems and model iron/silicon alloys were compared using Scanning Electron Microscopy (SEM), Energy Dispersive X-ray (EDAX) spectroscopy, and X-ray Photoelectron Spectrometry (XPS) sputter depth profiling. It was found that enhanced corrosion resistance was associated with underlying dramatic changes in corrosion layer composition and microstructure. From these observations, several possible mechanisms for the enhanced corrosion resistance were proposed.

To test these mechanisms:

1. It was suggested that some possible test samples be exposed in the DELTA loop (e.g. shot peened 316L) that are subsequently studied, along with other samples from the DELTA facility.
2. A high temperature lead-certified laboratory space (the High Temperature Materials Experiments Facility, HTMEF) was established where investigators are able to conduct molten LBE studies safely.
3. A Liquid Metal Corrosion Experiment (LMCE) is under construction, which will be a facility that allows the intro-



The High Temperature Materials Experimental Facility and Task 18 students and faculty.

duction, exposure, and extraction of materials test samples to hot (~1000°C) lead alloys (such as LBE) under careful atmospheric control. The facility will be made of refractory ceramics and metals, and thus will have better chemical control than steel based test systems. Lastly, it will be modular in design, allowing rapid changes to process parameters.

4. An existing mass selective ion beam apparatus is being upgraded to allow the implantation of isotopically labeled steel components into the samples, to allow monitoring of the diffusion of steel constituents in the corrosion layers and in the metal adjacent to the corrosion layers.
5. A set of gas phase experiments were started in sealed ampules and under controlled atmospheres to look at the formation of the corrosion layers and to track compositional changes in the corrosion layers and their substrates.

RESEARCH ACCOMPLISHMENTS

Effort 1: Shot-peened (i.e., *in situ* cold worked) 316L steel samples were studied that were exposed at the DELTA loop at LANL. Shot-peening with smaller beads improved corrosion resistance: the smoother surface had fewer and smaller failures (see the top figure on the opposite page). This argues against the mechanical “keying” mechanism that was proposed earlier to explain the improvements in corrosion resistance observed with cold rolled 316L. On the other hand experiments at the Environmental Molecular Sciences Laboratory using a scanning Auger microprobe did not see evidence of improved chromium coverage in the cold worked material.

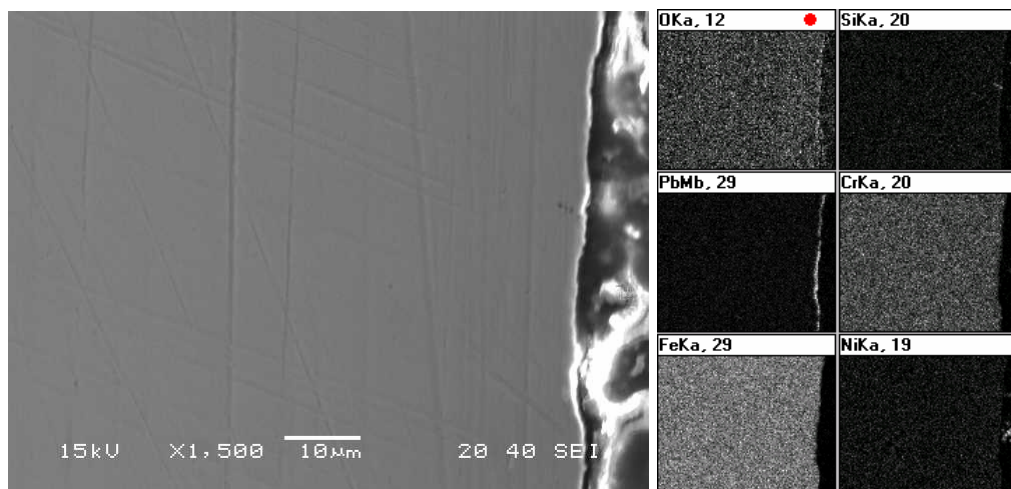
Effort 2: Plans were made to start experiments in the HTMEF (see figure on the previous page) in July 2005. The initial experiments will be gas phase experiments tracking the migration of alloy components during oxide growth at high temperature and low oxygen concentration.

Effort 3: The construction of the furnace section of the LMCE is essentially complete – while construction in the HTMEF continues.

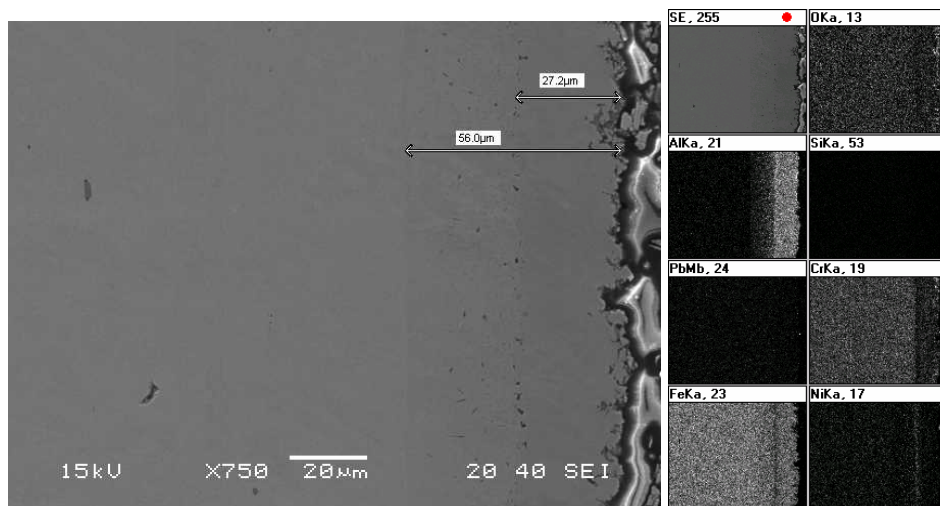
Effort 4: Aluminized 316L showed low corrosion but has a very complicated segregated surface/near surface region (see bottom

ACADEMIC YEAR HIGHLIGHTS

- ♦ “Application of X-ray photoelectron spectroscopy to the study of the lead-bismuth eutectic (LBE)-induced corrosion of stainless steel” by D.L. Perry, J.W. Farley, A.L. Johnson, D. Koury, B. Hosterman, U. Younas, and T. Ho was presented at a poster session at the ACS meeting in San Diego, March 13-17, 2005.



Shot-peened 316L exposed to LBE at the DELTA loop, LANL.



Aluminized 316L exposed to LBE at the DELTA loop, LANL.

figure). A paper is being prepared describing the effects of silicon in providing a protective layer. The aluminum results suggest that a significantly different protective layer may modify the underlying near-surface region in complicated ways. Ion beams have been obtained in the mass selective ion beam apparatus and the team is ready to start implanting stable isotopes to track diffusion in the metals and their oxides.

Effort 5: The required instrumentation will be delivered to UNLV in July 2005 to start the gas phase experiments. Initial experiments will use a multiple zone tube furnace to heat an evacuated quartz ampoule to two different temperatures: one end will hold the sample under test and the second side will hold mixtures of copper and copper oxide at temperature to set the oxygen concentration. Later experiments will investigate the addition of LBE to the oxidation conditions.

FUTURE WORK

The certification of the HTMEF for lead work and the completion of the LMCE will continue. An investigation of the migration of isotopically labeled components in the oxidation and corrosion of the test alloys will be initiated. Investigations of samples exposed in the DELTA loop will be continued.

Faculty

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 Allen Johnson, Assistant Professor, Department of Chemistry
 Dale Perry, Lawrence Berkeley National Laboratory; Adjunct Professor, UNLV Department of Physics

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 Thao Trung Ho, Graduate Student, Department of Chemistry

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Ning Li, LBE Project Leader, Los Alamos National Laboratory
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Task 19

Dissolution, Reactor, and Environmental Behavior of ZrO_2 -MgO Inert Fuel Matrix

K. Czerwinski

BACKGROUND

There has been a recent resurgence of interest in different oxide fuel types (Th, inert matrix, Pu fuel) as potential advanced fuel for Generation IV nuclear energy systems that can be operated to relatively high burnups at lower costs than current UO_2 fuels. These fuels can also be formed to incorporate transuranic elements in the matrix, acting as a host for these elements. Inert fuel matrices have the advantage of burning Pu and other transuranic elements from the fuel cycle without the production of other actinide elements. Of the possible materials for use in an inert matrix, ZrO_2 has been examined. The inclusion of ZrO_2 is expected to increase chemical stability and radiation resistance. The natural analogue of zirconia, baddeleyite ($(\text{Zr,M})\text{O}_2$), where M is a tetravalent ion such as hafnium), contains up to 3000 ppm uranium or thorium. This supports the durability of inert matrix fuels using ZrO_2 in reactor conditions and repository conditions. However, fuels appropriate for the advanced fuel cycle applications should have desirable reprocessing properties, namely ease of dissolution for separations. An additional oxide which is somewhat soluble may need to be added to the ZrO_2 matrix to achieve desirable reprocessing properties. A candidate oxide is MgO.

Inert fuel matrices containing a mixture of ZrO_2 and MgO have not been studied. It is proposed that such an inert fuel matrix will have reactor behavior and reprocessing properties desirable for an advanced fuel. This project will examine inert fuels containing ZrO_2 and MgO as the inert matrix. Ceramics with this inert matrix and U and Pu will be synthesized and examined. While the AFCI focus is on inert fuels with Pu as the fissile component, this task will perform laboratory experiments with both U and Pu. The initial work with U will be performed early in the project with results used as a basis for Pu studies. Reactor physics calculations will be used to examine suitable quantities of burnable poisons from the candidate elements Gd, Er, or Hf. Most fuels use Gd or Er, but the chemical properties of Hf lend themselves to formation of solid solutions with Zr and the tetravalent actinides and will therefore be investigated. The solubility of the fuel ceramics, in reactor conditions, reprocessing conditions, and repository conditions, will be investigated in a manner to provide

the necessary data for evaluating the performance, reprocessing, and waste behavior of the MgO-ZrO₂ fuels from a quantified, chemical perspective.

RESEARCH OBJECTIVES AND METHODS

This project examines inert fuels containing ZrO_2 and MgO as the inert matrix, with the relative amount of MgO varied from 30 % to 70 % in ZrO_2 . Reactor physics calculations are used to examine suitable quantities of burnable poisons from the candidate elements Gd, Er, or Hf with reactor grade Pu providing the fissile component, with up to 10 % of ^{239}Pu . Ceramics are synthesized and characterized based on the reactor physics results. The solubility of the fuel ceramics, in reactor conditions, reprocessing conditions, and repository conditions, are investigated in a manner to provide thermodynamic data necessary for modeling.

The research objectives of this project are as follows:

- To examine the neutronic behavior of MgO-ZrO₂ inert fuels. Variation of MgO and ZrO₂ composition ranges from 30 % to 70 % MgO in ZrO₂. Analysis of Gd, Er, and Hf for reactivity control ranging from 5-10 % lanthanides. Analysis of reactor grade Pu as fissile component ranging from 5-10 % Pu. Results will be used as parameters for fuel composition.
- To synthesize and characterize of MgO-ZrO₂ ceramics containing burnable poison and fissile composition. Synthesis is based on a precipitation method. Range of MgO in ZrO₂, Pu concentration, and burnable poison concentration based on results of neutronic calculations. Characterization of ceramics will include density, X-ray diffraction, surface area analysis, X-ray absorption fine structure spectroscopy, and chemical composition. Results will be applied to behavior in high temperature water, acid, and environmental conditions.
- To describe the chemical behavior of synthesized ceramics. Chemical thermodynamic and kinetic analysis will use equilibrium data, kinetic data, and surface area normalized dissolution. Different conditions will include reactor conditions (high temperature and high pressure water) and reprocessing conditions (nitric acid and elevated temperature). Environmental conditions will be near neutral solution conditions.
- To utilize project data in kinetic and thermodynamic modeling codes to evaluate the speciation of the elements in the ceramics under reactor, reprocessing, and repository conditions.

RESEARCH ACCOMPLISHMENTS

Ceramic Pellet Synthesis

The inert fuel matrix project is underway with progress in ceramic synthesis and pellet assembly. Zirconium oxide and magnesium oxide ceramics in varying ratios are synthesized from aque-



MgO-ZrO₂ pellets synthesized from precipitation of metal salts.

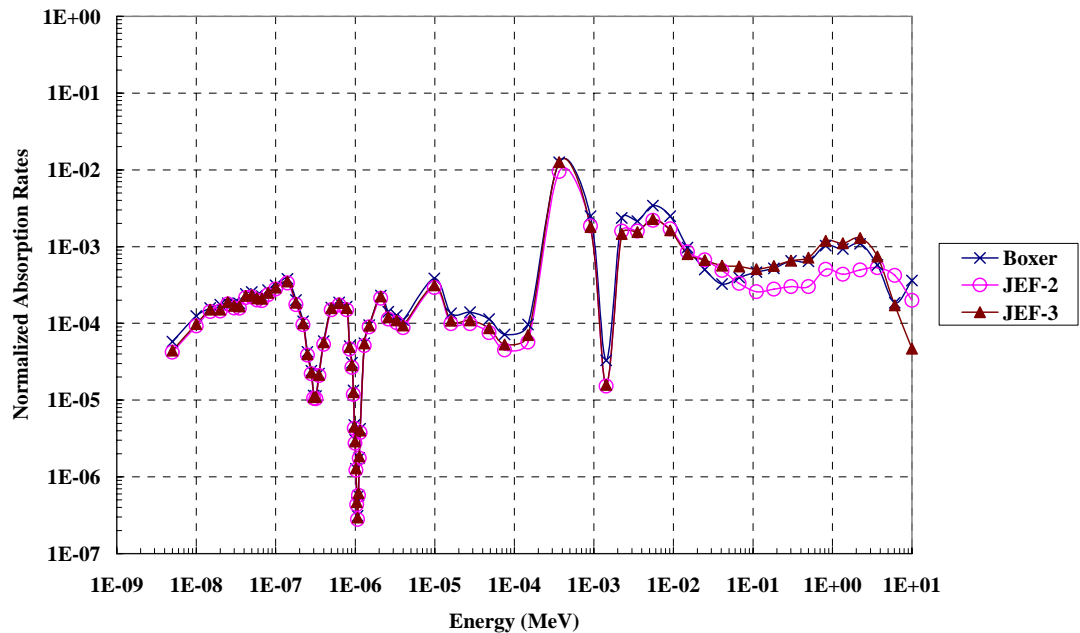
aqueous Zr^{4+} and Mg^{2+} ions prepared from zirconium chloride (ZrCl_4) and magnesium chloride hexahydrate ($\text{MgCl}_2 \cdot 6\text{H}_2\text{O}$), respectively. From this solution, hydroxides of these two metals are precipitated using ammonium hydroxide. The precipitate is filtered, ground to a powder, and calcined at 700°C for one hour to drive off the water of hydration. The product is zirconium oxide (ZrO_2) and magnesium oxide (MgO). Starting with ions in solution, precipitating out together will yield a higher probability of the final product being a zirconium oxide and magnesium oxide solid solution.

A pellet die was developed from a similar design used at Argonne National Laboratory – West. Powdered ceramics were pressed into pellets at pressures around 100 MPa using a laboratory press. The formed pellets were sintered at 1500°C for 4 hours under an argon atmosphere. Finished pellets were 1 cm by 1 cm diameter cylinders resembling nuclear fuel pellets (see figure on opposite page). Near term efforts will focus on characterization of existing pellets, synthesis of pellets with differing Zr:Mg ratios, and initial synthesis of uranium containing pellets.

Reactor Physics Calculations

A number of benchmark calculations for a standard PWR unit cell and 17×17 fuel assembly were performed with the code BOXER. BOXER is a modular code for two-dimensional neutron transport calculation of LWR fuel lattices.

The results of the BOXER computer code, suggested for use in the analysis of fertile free matrix fuels, were compared with MCNP results for different Pu loadings and cross section libraries. The criticality prediction difference between BOXER and MCNP ranges between 0.13 and 0.37% depending on the cross section library and Pu loading. The absorption rates in Zr, ^{240}Pu and ^{242}Pu isotopes were identified as major contributors to the discrepancy in criticality prediction. Relatively large Zr contribution to the total k-infinity prediction difference is due to the large Zr concentration in the fuel matrix as compared to a typical



Absorption rates in Zr in 70 energy groups.

UO_2 fuel where Zr is only present in the cladding. The relative error introduced by the Zr cross section data uncertainty decreases with an increase of Pu v/o and related hardening of the neutron spectrum (see figure above). This is expected to introduce additional uncertainty in evaluation of Moderator Temperature and Void reactivity feedback coefficients as pointed out in Baldi et al. (2001). Validation of BOXER computer code with respect to the accuracy of reactivity coefficients evaluation will be performed in the next stage. Analysis of the energy dependent differences for major isotopes presented in this report will provide a starting point for these studies.

The fuel assembly benchmark case tested the capabilities of 2D transport module of the BOXER code. Reasonable agreement in criticality prediction of the standard 17×17 PWR fuel assembly between BOXER and MCNP - on the order of 0.2% $\Delta\rho$ was observed. The fuel assembly local pin power distribution predicted by the two codes is within 2% discrepancy.

In conclusion, the performed benchmark calculations confirmed that the BOXER code is suitable for the scoping studies of plutonium in fertile free matrix fuel designs. The BOXER code predicts criticality, reaction rates and power distribution in fuel assembly with accuracy sufficient for the purposes of this study.

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Task 20

Effect of Silicon Content on the Corrosion Resistance and Radiation-Induced Embrittlement of Materials for Advanced Heavy Liquid Metal Nuclear Systems

A.K. Roy

BACKGROUND

Recent studies at the Los Alamos National Laboratory (LANL) involving martensitic Alloy EP-823 containing different silicon content have revealed a beneficial effect of Si on corrosion resistance in a molten lead-bismuth-eutectic (LBE) environment. Since very little data exist in the open literature on the beneficial effect of Si on the corrosion resistance of martensitic alloys, a research task was initiated to explore the role of Si not only on the corrosion resistance but also on the radiation-induced embrittlement of martensitic stainless steels.

This task is focused on the evaluation of the effect of Si content on the corrosion behavior and radiation-induced embrittlement of martensitic steels having chemical compositions similar to that of modified 9Cr-1Mo steel. Numerous state-of-the-art experimental techniques are currently being planned to be employed to achieve the desired research goal.

RESEARCH OBJECTIVES AND METHODS

Four different experimental heats of ASTM A 213 Type T91-grade alloy steels (similar to Mod9Cr-1Mo) with different Si content (0.48, 1.02, 1.55 and 1.88 weight percent) have been melted by the vacuum-induction-melting practice at the Timken Re-



Corrosion-resistant autoclave.



INSTRON high-temperature mechanical properties testing machine.

search Laboratory. They were subsequently processed into rectangular and square bars by forging and hot-rolling. These bars were then austenitized, oil-quenched, and tempered to achieve fine-grained and fully-tempered martensitic microstructure. Machining of different types of specimens from these heat-treated bars is ongoing.

Tensile properties of all four heats will be evaluated both at ambient and elevated temperatures by using cylindrical specimens according to the ASTM Designation E 8. Micro-structural evaluations will be performed by optical microscopy. In order to study the effect of radiation on the tensile properties and impact resistance of the test materials, both cylindrical and Charpy V-notch specimens will be used.

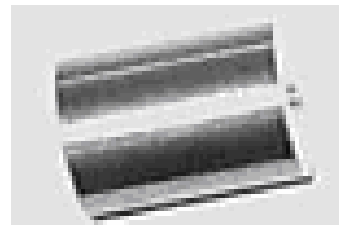
The tensile specimens will enable a comparison of mechanical properties including the yield strength (YS), ultimate tensile strength (UTS), percent elongation (%El) and percent reduction in area (%RA), with and without radiation. The notched Charpy specimens will enable the determination of the impact energy as a

function of temperature, and the ductile-to-brittle transition temperature (DBTT) as functions of the Si content and the radiation dose. The morphology of failure on the tested cylindrical and Charpy specimens will be determined by scanning electron microscopy (SEM). Transmission electron microscopy (TEM) will be used to characterize the defects during plastic deformation as a function of temperature.

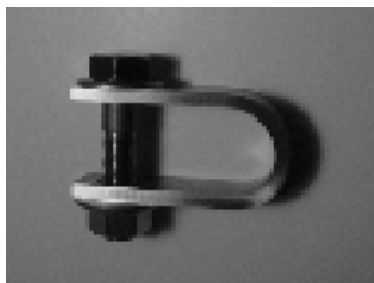
The general and localized corrosion behavior of all four heats of T91-grade material will be determined by using rectangular coupons. The susceptibility to stress corrosion cracking (SCC) will be evaluated by using tensile and self-loaded C-ring and U-bend specimens in both LBE and aqueous environments. SCC testing using cylindrical specimens will be performed in aqueous environments either at constant load (CL) or under a slow-strain-rate (SSR) condition. The C-ring and U-bend specimens will be tested in an autoclave in the presence of an aqueous solution at temperatures up to 650°C. The localized corrosion (pitting and crevice) tendency will be studied in an aqueous solution by cyclic potentiodynamic polarization (CPP) technique. The CPP test will determine the corrosion potential (E_{corr}), critical pitting potential (E_{pit}), and the protection potential (E_{prot}), if any. Fractographic evaluations of all SCC test specimens will be performed by SEM.



Tensile (Smooth & Notched)



Polarization



U-Bend



C-Ring

Test specimens.

FUTURE WORK

It is anticipated that this task will lead to the development of the following scientific/technical information:

- Metallurgical microstructures as functions of Si content and radiation dose.
- Tensile properties (YS, UTS, %El and %RA) before and after radiation.
- Impact resistance (impact energy and DBTT) versus Si content and radiation dose.
- Failure stress, ductility (%El and %RA), and threshold stress for SCC.
- Liquid-metal-embrittlement versus Si content.
- General corrosion rate versus Si content and temperature.
- E_{corr} , E_{pit} and E_{prot} versus Si content and temperature.
- Effect of hydrogen on SCC through controlled potential versus Si content.
- Extent and morphology of cracking (ductile/brittle, intergranular/transgranular).
- Voids due to radiation damage.
- Understanding the effect of Si on the metallurgical and corrosion behavior of T91-grade steels.

Research Staff

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Task 21

Theoretical Modeling of Protective Oxide Layer Growth in Non-isothermal Lead Alloy Coolant Systems

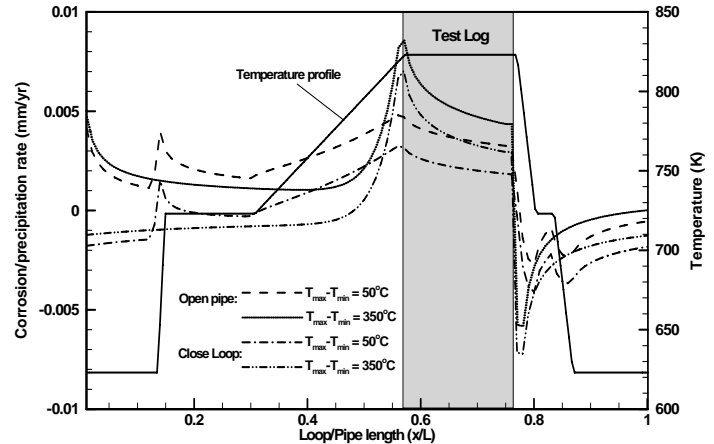
Y. Chen, J Zhang, H. Chen, J. Li

BACKGROUND

In advanced nuclear energy systems, lead-alloys (e.g., lead, lead-bismuth eutectic) emerge as strong candidates for transmutation and advanced reactor systems as nuclear coolants and high-power spallation neutron targets. However, it is widely recognized that corrosion of materials caused by lead-alloys presents a critical barrier to their industrial use. A few experimental research and development projects have been set up by different groups such as LANL to study the corrosion phenomena in their test facilities and to develop mitigation techniques and materials.

One of the central or main techniques in lead-alloys coolant technology under development is to use active control of oxygen thermodynamic activity (OTA) to provide protective oxide layers. Setting OTA in flowing lead-alloys makes corrosion highly dependent upon the oxygen concentration and the oxidation processes at materials surfaces. The active oxygen control technique exploits the fact that lead and bismuth are chemically less active than the major components of steels, such as Fe, Ni, and Cr. By carefully controlling the oxygen concentration in LBE, it is possible to maintain an iron and chrome based oxide film on the surfaces of structural steels, while keeping lead and bismuth from excessive oxidization that can lead to precipitation contamination. Thermal analysis has given an ideal oxygen level range in a non-isothermal lead-alloys coolant system. However, in a practical coolant loop, the proper oxygen level depends not only on thermal factors but also on hydraulic factors (system operating temperature, temperature profile, flow velocity, etc.). In addition, the oxygen distribution in a non-isothermal lead-alloys coolant system is still unclear. The optimal oxygen levels still need to be investigated.

The goal of the proposed research project is to provide basic understanding of the protective oxide layer behaviors and to develop oxide layer growth models of steels in non-isothermal lead-alloys (lead or lead-bismuth eutectic) coolant systems. Precise studies and simulations of all hydrodynamics with thermal conditions encountered in practical coolant loop systems by use of different flowing conditions in the laboratory are difficult and expensive, if not impossible. Therefore it is important and necessary to develop theoretical models to predict the protective oxide layer behaviors at the design stage of a practical lead-alloy coolant system, to properly interpret and apply experimental results from test loops, and to provide guidance for optimization in lead-alloys nuclear coolant systems. The research project, therefore, is aimed at filling the gaps of protective oxide layer growth and the oxygen concentration level before lead-alloys nuclear coolant is ready for programmatic implementations and industrial applications.



Corrosion rate under different axial temperature distributions.

RESEARCH OBJECTIVES AND METHODS

The research objectives are:

- To elucidate the mechanism of the protective oxide layer growth of steels in static, non-isothermal flowing lead-alloys coolant systems with oxygen concentration level control.
- To elucidate the mechanism of mass transport of oxygen, corrosion products in the multi-phase system.
- To develop oxidation growth models of steels in lead-alloy coolant systems.
- To clarify the dependence of oxidation process on the hydraulic factors (system operating temperature, temperature profile, flow velocity, etc) and the oxygen concentration distribution and level.
- To clarify the optimal oxygen concentration levels in practical coolant system scales.
- To interpret the experimental results from test loops and to apply them to the design of practical nuclear coolant systems.

The research goals are:

- To understand the difference in oxidation behaviors between different types of structure materials.
- To incorporate the present oxide layer growth model to our previous kinetic corrosion model.
- To develop a general numerical code that can predict the oxygen concentration level, the oxidation growth rate and the corrosion rate in practical lead-alloys coolant systems.

Kinetic Model

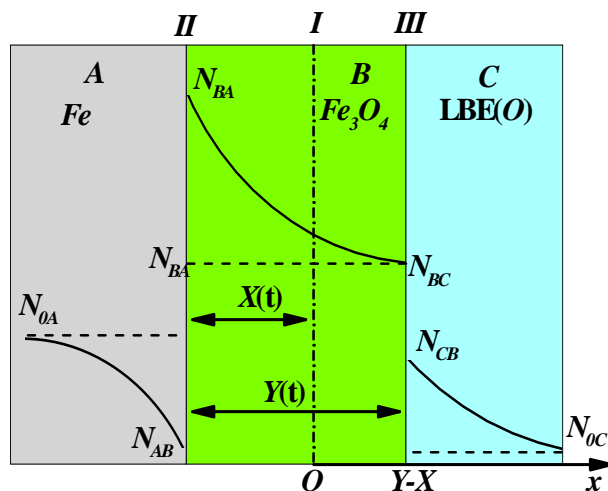
An improved kinetic model was developed to predict the mass transfer controlled corrosion/precipitation in non-isothermal LBE pipe/loop systems. Two sets of mass transfer equations were solved separately both in the turbulent core region and sub-layer region. The improved model was applied to the DELTA loop at Los Alamos National Laboratory. The DELTA loop is a non-isothermal closed loop and is used to study the corrosion of various materials in the flowing LBE system. The temperature profile is shown in the figure on the opposite page. This figure also shows the predicated corrosion/precipitation rate by the present model in the pipe/loop flow in the DELTA Loop. From this figure, one can find that there also exists a precipitation region in the open pipe case and this precipitation region occurs beside the highest temperature region because of the large axial temperature difference.

Numerical Analysis

Numerical analysis of the coupled natural convection and corrosion product transfer in a two-dimensional circular loop was made to study the corrosion product under the active oxygen controlled model.

Kinetic Oxide Growth Model

A kinetic oxide growth model in Liquid LBE was developed for the pure iron exposed liquid LBE with oxygen controlled. A schematic plot is shown in the figure below. The oxide Fe_3O_4 layer grows toward both in internal side (II surface) and external



Schematic plot of the structure of pure iron exposed to LBE with oxygen controlled. A region: Metal Fe; B region: Metal oxide Fe_3O_4 ; C region: Liquid LBE with oxygen; I: Original metal surface; II: Metal-oxide Interface; III: Oxide-LBE interface. X: Depth of metal consumption; Y: Width of Oxidation Layer.

ACADEMIC YEAR HIGHLIGHTS

- ◆ “Corrosion behaviors of U.S. steels in flowing lead–bismuth eutectic (LBE)” was published in *Journal of Nuclear Materials*, 2005,336, 1–10.
- ◆ “Oxidation Mechanism of Steels in Liquid–Lead Alloys,” was published in *Oxidation of Metals*, 2005, 63, 353-381.
- ◆ “Modeling corrosion and precipitation in non-isothermal LBE pipe/loop systems,” was submitted to *Journal of Nuclear Science and Technology*, 2005, in press.
- ◆ “Dynamics of high-temperature oxidation accompanied by 3 scale removal and implications for technological applications,” was submitted to *Journal of Nuclear Materials*, 2005, in press.
- ◆ “A improved Kinetic Corrosion Model in Non-isothermal loop/pipe Systems,” was presented at the ANS Student Conference, Columbus, OH, April 14-16, 2005.

side (III surface). The following assumptions were made:

- The interfaces are local equilibrium and the processes do not affect the kinetics of oxidation.
- The growth of the oxide Fe_3O_4 is limited by the diffusion of iron.
- The diffusion of oxygen anion is neglected.
- The oxide layer growth and the consumption of metal obey the Wagner’s parabolic law.
- The interfaces are flat plat.

FUTURE WORK

The next phase of the project involves accomplishing the following tasks:

- Illustration of the oxidation process mechanisms in oxygen control lead-alloys systems.
- Identification of the protective oxide layer growth rate and the dependence on the thermal and hydrodynamic factors of the entire coolant loop.
- Optimal operation conditions for oxygen control lead-alloys systems.
- Analytical models for various limiting process regimes.
- Development correlations and tools for calculations of the oxidation rate, oxygen concentration level and distribution, and oxygen consumption.

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Task 22

Design Concepts and Process Analysis for Transmuter Fuel Manufacturing

G. Mauer

BACKGROUND

The safe and effective manufacturing of actinide-bearing fuels for any transmutation strategy requires that the entire manufacturing process be contained within a shielded hot cell environment. To ensure that the fabrication process is feasible, the entire process must be designed for remote operation. The equipment must be reliable enough to perform over several decades, and also easy to maintain or repair remotely. The facility must also be designed to facilitate its own decontamination and decommissioning. In addition to these design factors, the potential viability of any fuel fabrication process will also be impacted by a number of variables, such as the current state of technology, potential problem areas, deployment scaling, facility safety, and cost.

RESEARCH OBJECTIVES AND METHODS

The goal of this research project is to provide technical support to process designers working on the development of the fuel cycles for transmutation applications. Detailed process models have been developed to better define the impact of fuel choice on the transmuter fuel cycle, including relative process losses, waste generation, and plant capital cost. These process models provide insight regarding required plant size and number of plants needed to mesh with the fuel recycling line. They also determine requirements for automation.

Manufacturing models for large-scale production in a hot cell environment have also been developed. Combined, these two models allow the assessment of plant layout, and provide the framework for estimation of plant capital and operating cost esti-

mates, and for feasibility in general. The operations of robotic equipment and the sensor technology required for safe and reliable robot control have been evaluated through simulations in three-dimensional space. The manufacturing technology developed for hot cell applications is also applicable to other, more general uses, where occupational hazards prevent human presence near processes.

The research work was divided into several tasks:

Conceptual 3D modeling: Hot Cell Robotics and Equipment Simulation – A literature survey and detailed analysis of the research and development pertaining to candidate processes for transmuter fuel manufacture continued from previous years. Industry standards were used to refine equipment, instrumentation, and control specifications, and assessed the reliability and safety of operations. Monitoring of the market continued for equipment and components, which were evaluated with regard to suitability for automated manufacturing under hot cell conditions.

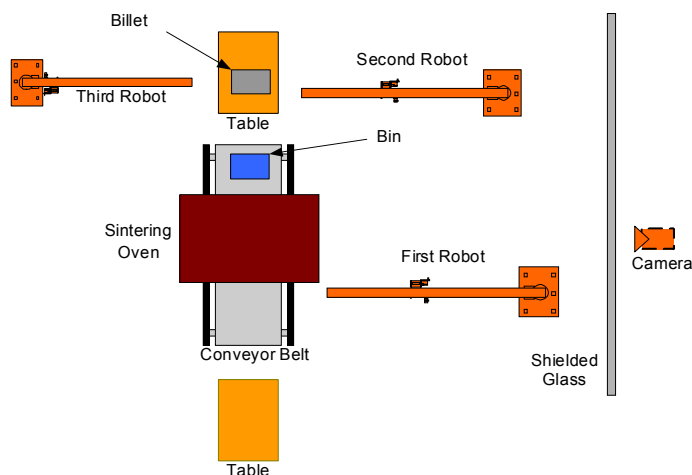
Simulations – This task modeled manufacturing processes to generate a realistic assessment of plant layout, size, feasibility, and technology development required for large-scale remote fabrication of fuel. Modeling of the candidate fuel manufacturing processes was performed using the MSC.visualNastran and ProEngineer simulation software tools. The modeling of dispersion and TRISO fuels has been completed. A parametric study to determine the process reliability and possible reliability improvements for various fuel types and equipment configurations is ongoing.

Cost, Feasibility, and Large Scale Deployment – This task developed the database necessary to provide cost estimates and differential cost for various fuel manufacturing options. Efforts began to tabulate and quantify estimates regarding projected cost, reliability, and plant life.

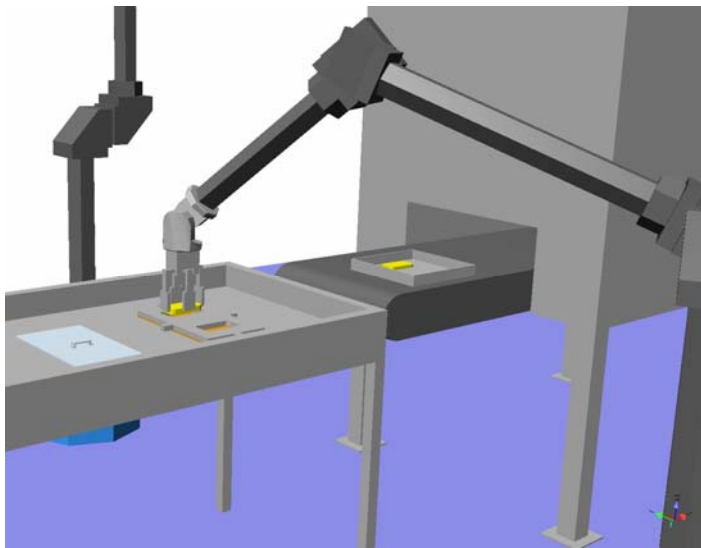
RESEARCH ACCOMPLISHMENTS

A simulation model with a Waelischmiller hot cell robot was developed and coupled with MatLab control software. Matlab provides the interface with the robot and is used to control the system. The simulation renders a realistic simulation of the forces and torques present during robot motion. A 3-D manufacturing process simulation using CAD models and the Newtonian dynamics of the moving components has been developed.

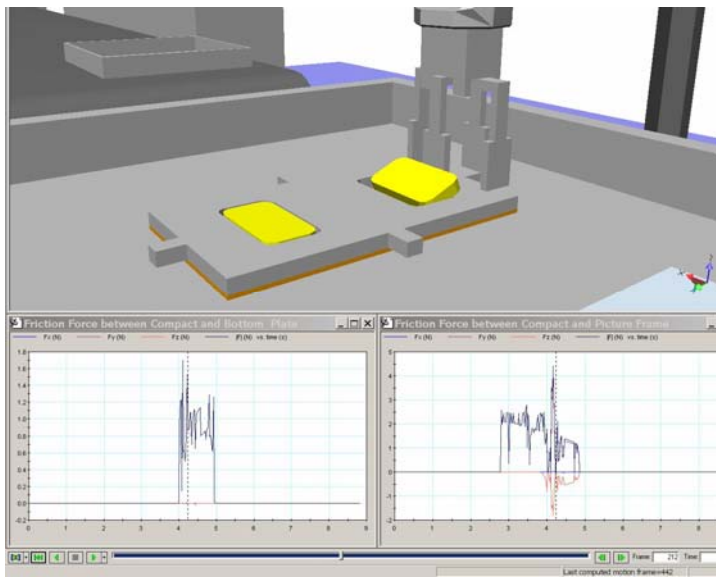
When designing and analyzing operations inside a hot cell, considerable efforts are usually devoted to mockup studies that seek to anticipate both normal operations and accidents. The Visual



Schematic of the floor layout of a hot cell manufacturing dispersion fuel.



Dispersion Fuel Manufacture: Manipulator placing a sintered compact into the billet.



Dispersion Fuel Manufacture: Friction forces between compact and cladding during insertion into the billet

Nastran models represent a virtual mock-up facility, in which multiple accident scenarios were examined and analyzed in detail.

Results exist in the form of movies, data sets, and images. Simulations for six-axis Wälischmiller robots were developed and their proper kinematic configuration was verified. The simulations permit the detailed analysis of forces and torques in any modeled part or component.

ACADEMIC YEAR HIGHLIGHTS

- ◆ “Conceptual Workcell Design and Throughput Analysis for Robotic Transmuter Fuel Fabrication,” by G.F. Mauer and J. Renno was published in the Proceedings of the ANS Winter Annual Meeting, November 2004.
- ◆ “Design Concepts and Process Analysis for Transmuter Fuel Manufacturing,” by G.F. Mauer was published in the Proceedings of the 8th Partition in a Transmutation Information Exchange Meeting, OECD Nuclear Energy Agency, Las Vegas, NV, November 2004.
- ◆ Jamil Renno completed and defended his M.Sc. thesis in Mechanical Engineering (March 2005). Thesis title: “Virtual Design and Modeling of Various Manufacturing Processes for Remote Fuel Fabrication of Transmuter Fuel.”

The simulations are numerically extensive, and a single simulation can require hours to complete, depending on the complexity of the model. The speed of the simulation has been increased substantially through continuous equipment upgrades, which were essential in enabling more detailed model refinements without undue elongation of simulation run times.

FUTURE WORK

Further efforts will be devoted to increasing data and knowledge regarding the cost and feasibility of automated fuel manufacture in a hot cell by analyzing candidate manufacturing processes. Artificial intelligence concepts will be developed further with respect to object identification and hot cell dynamics simulations. Failure scenarios are being analyzed with regard to plant reliability, and the introduction of redundant equipment and sensors for the purpose of increasing plant reliability. A literature study to retrieve failure and reliability data is under way. The placement of robots in the hot cell is being evaluated with regard to optimizing their capability for redundancy in the event of equipment failure or maintenance.

A visit of the MELOX plant in Marcoule is planned for July 2005 with the objective of gaining insights into the design and operations experience gained from an operational plant.

The results of the simulations will be used by AFCI program personnel to perform sensitivity studies on the impact of different fuel types on transmutation system operation. Conceptual designs of the fuel fabrication processes will allow evaluations of issues related to maintainability, robust design, and throughput rate, and lead to identification of areas where improvements in technology are required to meet the goals of the transmutation system.

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Task 23

Development of Nanostructure Based Corrosion-Barrier Coatings on Steel for Transmutation Applications

B.J. Das

BACKGROUND

Advanced transmutation systems require structural materials that are able to withstand high neutron fluxes, high thermal cycling, and high resistance to chemical corrosion. The current candidate materials for such structures are ferritic and ferritic-martensitic steels due to their strong resistance to swelling, good microstructural stability under irradiation, and the retention of adequate ductility at typical reactor operating temperatures.

In parallel, lead bismuth eutectic (LBE) has emerged as a potential spallation target material for efficient production of neutrons, as well as a coolant in the accelerator system. While LBE has excellent properties as a nuclear coolant, it is also highly corrosive to stainless steel. The corrosion is due to relatively high solubilities of the base and major alloying components of steel, such as Ni, Fe, Cr, etc. in LBE at elevated temperatures. Without some protection, the steel structures rapidly corrode in LBE through dissolution and leaching of these materials.

Thus, for long term reliability of the structures, it is necessary to provide some protection of the steel surface from corrosion, without affecting the bulk properties of the steel. One such technique that has been well investigated is the use of oxygen control at the surface of the steel, which maintains a coating of oxide layer that protects the steel surface. The protective layer forms due to the higher affinities of the steel alloying components to oxygen compared to lead and bismuth. However, once a continuous film of oxide is formed, a competing process takes place; the oxide layer interacts with the LBE causing reduction of the oxide layer at higher temperatures. It is thus critical to maintain an optimum flow of oxygen at the LBE/steel interface, which is made challenging by the non-uniform temperature distribution in the transmutation systems. In addition, while the oxygen control technique works effectively at lower temperatures, it is not appropriate for

higher operational temperatures (500-600°C), which is becoming increasingly important. Thus, it is necessary to develop alternative techniques for corrosion protection of steel that will perform reliably at elevated temperatures and under thermal cycling in LBE.

RESEARCH OBJECTIVES AND METHODS

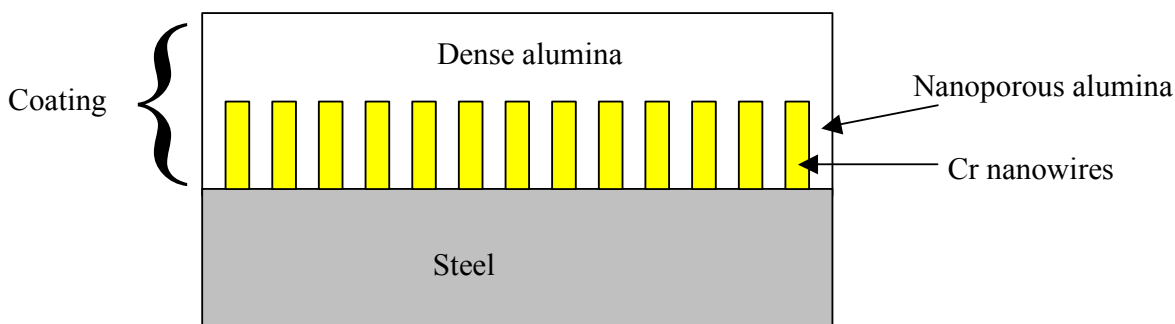
The objective of this project is to develop a novel nanostructure based coating technology that will provide significantly improved corrosion resistance for steel in LBE at elevated temperatures (500-600°C), as well as provide long-term reliability under thermal cycling. The nanostructure based coatings will consist of a layer of nanoporous alumina with the pores filled with an oxidizing metal such as Cr, followed by a capping layer of alumina. Alumina, which is a robust anti-corrosion material, provides corrosion resistance at elevated temperatures. The Cr serves two purposes: (1) it acts as a solid filler material for the pores in the alumina, enhancing its mechanical and chemical integrity, and (2) it acts as a second layer of defense against corrosion by providing a replenishable source of Cr (for the formation of a Chromium oxide protective layer) in case the alumina layer is compromised. The innovation of this project is the use of a nanoporous alumina layer for the coating, which is mechanically flexible and can expand and contract with the underneath steel surface. As a result, the mechanical integrity of the coating is preserved under thermal cycling. In addition to their usefulness at higher temperatures, the proposed coatings can also provide increased reliability at lower temperatures by complementing the oxygen control technique. The nanostructure based coatings developed in this project will significantly enhance the long-term reliability of steel structures in LBE at elevated temperatures and under thermal cycling.

Working with the DOE collaborator, the stainless steel alloys HT-9 and EP-823 were chosen as the candidate materials for investigation at this time. The above project objective will be achieved in three phases; each phase will be carried out over a one-year period.

Phase I will develop the fabrication technology for the coatings on steel, and study their structural integrity at elevated temperatures and under thermal cycling.

Phase II will perform corrosion studies of the structures in LBE at elevated temperatures.

Phase III will use the data from Phases I and



Schematic cross-section of the proposed nanostructure based coating. The nanoporous nature of the bottom alumina layer allows it to expand and contract with the steel surface thus preserving the mechanical integrity of the coating under thermal cycling. The dense alumina layer, provides the first layer of protection against corrosion. The Cr nanowires, in addition to enhancing the structural and chemical integrity of the nanoporous alumina, provides a second layer of protection in case the alumina layer is compromised. Stacked multiple layers of the coating structure can be created on steel surface to provide increased protection against corrosion.



Photograph of two anodized samples showing the porous alumina on steel.

II to develop an optimized coating technology for improved structural integrity under thermal cycling, and improved corrosion resistance in LBE at elevated temperatures. If necessary, multiple layers of such coating structures will be used for increased resistance to corrosion.

The following are the specific goals this year for the project:

- To develop the technology to create thick nanoporous alumina layers on HT-9 and EP-823 steel.
- To electrochemically deposit Cr nanowires inside the alumina pores.
- To develop the technology to create thick dense alumina layer on top of the Cr nanowires.
- To investigate the structural integrity of the coatings at elevated temperatures and under thermal recycling.

RESEARCH ACCOMPLISHMENTS

A specialized sample holder was developed for the anodization of alumina on steel. In addition, it was determined that oxalic acid was the most appropriate acid for the anodization of these structures. The steel samples obtained from LANL were first cut into a number of pieces, each measuring 11mm x 8mm x 1.6mm, to allow multiple experiments.

The steel samples were cleaned and a thin layer of titanium (10 nm thick) was deposited on the surface of the steel followed by deposition of a thick layer of 99.999% aluminum (1 μ m thick) using e-beam evaporation. The Ti layer was deposited for improved adhesion of aluminum on steel; direct deposition of aluminum on steel showed poor adhesion. The samples were then anodized in 0.3M Oxalic acid solution maintained at 15°C using a constant current density of 20mA/cm². Visual inspection of the samples (shown in the figure above) also confirmed the formation of the porous alumina layer. The samples were then coated with a thin layer of gold and characterized by SEM imaging. However, the surface of the sample was found to be very rough, which made high resolution imaging very difficult.

ACADEMIC YEAR HIGHLIGHTS

- ♦ Adhesion properties of thin film nanoporous alumina templates” was submitted by to the *J. Vacuum Science & Technology* (in review).
- ♦ “Nanostructure Based Corrosion-Barrier Coatings on Steel for Transmutation Applications,” was presented at the ANS Student Conference, April 2005, Columbus, OH (received 2nd best paper award).
- ♦ “Template based Nanofabrication: Mechanical Characterization of Film-substrate Interface” was presented at the 3rd International Conference on Experimental Mechanics, Singapore, Nov. 29-Dec. 1, 2004.
- ♦ “Nanostructure based Composite Material Coatings on Steel” by B. Das and P. Singaraju was presented at the Int. Conf. Adv. Composite Mat (ICRACM-2004), Varanasi, Dec. 17-19, 2004.

An important requirement for this project is good adhesion of the coating film on the substrate under thermal cycling. Towards this goal, the samples were subjected to thermal cycling to 300°C and 400°C. Visual inspection of the samples showed the appearance of thermally cycled samples was the same as the uncycled (room temperature) samples. Also, a preliminary scratch test using a pin showed the alumina coating to have good adhesion to steel after thermal cycling.

FUTURE WORK

The next phase of the project will focus on (i) appropriate sample preparation to enable SEM imaging, (ii) thermal cycling to higher temperatures, (iii) deposition of Cr nanowires, (iv) formation of dense top alumina layer, and (v) characterization of the nanoporous coatings. While in the earlier alumina coatings the presence of nanopores could be confirmed, the samples were difficult to image due to surface roughness. To overcome this problem, nanoporous alumina coatings will be fabricated on polished steel surface. The steel samples will be polished mechanically as well as electrochemically followed by the deposition of aluminum. The nanoporous coatings on steel substrates will be subjected to elevated temperature thermal cycling, up to 500°C and 600°C. As before, the adhesion properties of the nanoporous alumina films will be evaluated using scratch tests.

Cr will be deposited inside the alumina nanopores electrochemically to form the Cr nanowires. Next, a dense layer of alumina will be formed on the surface through the hydration technique. If the hydration technique proves to be inadequate to form a sufficiently thick dense alumina layer, sputtering technique will be used to form such layers. The coating layers will be characterized next using scratch tests under different thermal cycling conditions.

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Task 24

Development of Integrated Process Simulation System Model for Spent Fuel Treatment Facility (SFTF) Design

Y. Chen and S. Hsieh

BACKGROUND

This effort is a continuation of the work of Task 8 (see page 20), and the same overview applies. The chemical separation process is calculated by the Argonne Model for Universal Solvent Extraction (AMUSE) code, developed in the 1980s, that designs multi-stage countercurrent flowsheets for the TRUEX solvent extraction process. The Generic TRUEX Model (GTM) and AMUSE predicts chemical behavior in solvent extraction processes by calculating component distribution ratios. Further, the counter-current mass balance algorithm contains terms for stage efficiency and other-phase-carryover for both the aqueous and organic phases. All five process segments of the UREX+ process were programmed into AMUSE code. The currently developed TRPSEMPro (Transmutation Research Project System Engineering Model PROgram) by the Nevada Center for Advanced Computational Methods (NCACM) at the University of Nevada-Las Vegas can be highly integrated with the AMUSE code and commercial packages to calculate the complex interactions between proposed process changes.

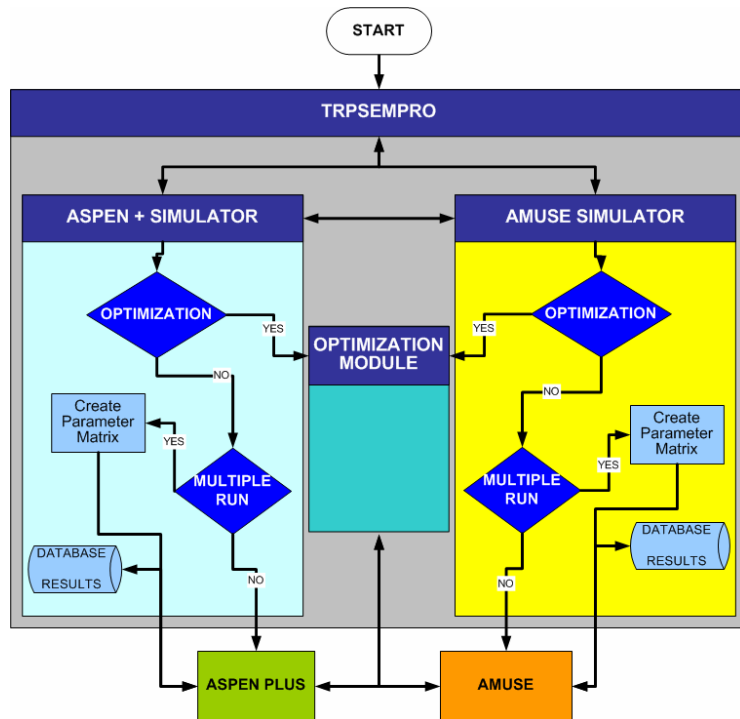
While successfully embedding AMUSE module into a dedicated System Engineering Model (TRPSEMPro), Argonne National Laboratory is interested in further simulating the Light Water Reactor (LWR) Spent Fuel Treatment Facility (SFTF) combining commercial process simulation packages and core calculation of the AMUSE that derived for using with the UREX+ process. The designed SFTF will receive, temporarily store, and prepare spent nuclear fuel for leaching. The leached fuel will then be separated by solvent extraction to recover:

- Uranium, Technetium and Iodine for disposal as low-level waste (LLW)
- Cs/Sr for decay storage and eventual disposal as LLW while Pu/Np for production of mixed-oxide (MOX) fuel
- Am/Cm for short-term storage and eventual use as fast-reactor fuel
- Two raffinates from the UREX+ process containing all soluble fission products but Cs, Sr, Tc, I, and the rare earth elements will be converted to a solid for disposal in the repository.

RESEARCH OBJECTIVES AND METHODS

The major objective is to create a framework that combines all the strengths of AMUSE's complicated calculations, well-established commercial system process package such as ASPEN-PLUS, HYSYS and PRO/II and TRPSEMPro's flexible parameter optimization modules. Development of the process simulation code can be done using the solvent extraction process experience at Argonne National Laboratory and in collaboration with the NCACM. The major activities of the task are the following:

- Develop a framework for simulating the SFTF process using AMUSE code, commercial process package, such as AS-



The framework design for the chemical separation process.

PEN-PLUS, and system engineering model.

- Develop a middleware package that can communicate between the AMUSE code and any selected commercial packages.
- Extend the existing system engineering model for optimization process that includes process simulation results.
- Include a scenario-based database system that efficiently reports required information as chart output using web-based programming, and Microsoft Visual Basic (MS VB).

A comprehensive study of commercial simulation packages has been performed by the Argonne National Laboratory. The three most promising packages identified were ASPEN-PLUS, HYSYS and PRO/II. All these packages require purchasing the aqueous electrolyte package that can incorporate AMUSE as the unit operation for solvent extraction. Since the ASPEN-PLUS provides a greater capability for solids handling, the major task here will create a communication tool between the AMUSE code and the ASPEN-PLUS. ASPEN-PLUS or an alternative, used for the SFTF process simulation, will be thoroughly studied for data parsing capability.

The NCACM team intends to develop a middleware package that can communicate between the AMUSE code and any selected commercial packages. An interface will be developed that incorporates AMUSE as the solvent extraction unit operation and any commercial package as the head-end and back-end processes.

RESEARCH ACCOMPLISHMENTS

This project identified the parameter correlations and data manipulation channels between the AMUSE code and the selected process simulation software package such as identified AMUSE input/output (from AMUSE Macros) to specify input streams associated with typical spent fuel, determine all inputs and outputs for each process block, select key components to monitor throughout process, and document key individuals or organizations for each process block. Also, AMUSE input/output (from TRPSEMPPro package) have been identified to specify input streams associated with typical spent fuel, determine all inputs and outputs for each process block, and select key components to monitor throughout process. The communication protocols from the selected process simulation package have also been identified to specify the possible data manipulation routes, determine the most suitable channel for data transferring, and streamline the discrepancies among AMUSE code, TRPSEMPPro and the selected process package such as ASPEN-PLUS, HYSYS and PRO/II.

The middleware for data manipulation among the AMUSE code, system engineering model and the selected process simulation software package has been developed to define Framework Architecture. The middleware has included a database design for temporary data repository. The XML data communication standard has been used for data manipulation. However, some of the process package might not support XML-enabled transfer and will be considered respectively. The middleware implementation – use programming languages, such as MS VB and VB.net, are under development.

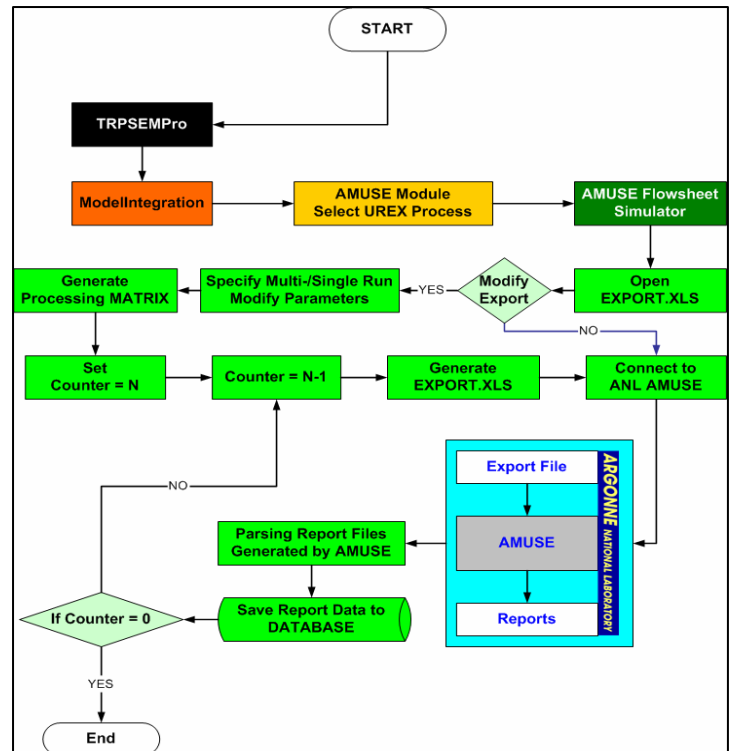
The overall TRPSEMPPro system model is evolving as the TRP project continues. UNLV will work to incorporate changes to the overall process as time advances and make changes to the software that allows it to be used as a part of the overall systems engineering model and that allows it to be used as a stand-alone process model. A few modifications need to be studied to allow the optimization of the process. Argonne National Laboratory collaborators will provide the system information to analyze a variety of proposed configurations.

FUTURE WORK

It could take years before incorporating all of the UREX separation processes into the developed systems engineering model. While waiting for completing the processes, developing more system analysis modules for TRPSEMPPro will definitely strengthen its capability on solving complex chemical separation process. Future work also includes increasing the sophistication of the systems engineering model, such as addition of optimiza-

ACADEMIC YEAR HIGHLIGHTS

- ♦ “Development of Systems Engineering Model for Spent Fuel Extraction Process” was published in the Proceedings of IMECE2004, ASME International Mechanical Engineering Congress, Anaheim, CA, November 13–19, 2004



Middleware design flowchart for the AMUSE Simulator.

tion tools. As optimization constraints are provided, relative comparisons of process options with regard to waste generation, proliferation resistance, throughput capabilities, facility requirements, and cost are possible. The system model will provide engineers and scientists a user-friendly Window-based graphical user interface package. Increased confidence in the models and further refinements render greater objectivity and technical credibility to the decision-making process. Also, three candidate software packages have been identified: Aspen Plus[®], HYSYS[®], and PRO/II[®], which will be coupled or interacted with TRPSEMPPro and AMUSE to define actinides and fission product physical-chemical databases, accurately predict aqueous electrolyte systems, and create a thermodynamic package for phase diagrams and coupling of phase diagrams with kinetic process modeling.

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Task 25

Electrochemical Separation of Curium and Americium

D.W. Hatchett and K. Czerwinski

BACKGROUND

In the AFCI program the separation of the trivalent actinides Am and Cm from the trivalent lanthanides, and even each other, has been identified as an area of particular interest. The removal of the lanthanides from the trivalent actinides is necessitated for neutron economy of a fuel containing Am and Cm. Furthermore, a fuel containing only Am would ease the demands on a reactor for transmutation. The destruction rate of Cm isotopes in a reactor is comparable to their decay rate. Separation and storage of the Cm, and reintroduction into the fuel as the Pu daughters is a transmutation option that can be explored if a suitable method for the separation of Cm from Am is obtain. Furthermore removal of Cm would reduce difficulties in fuel fabrication.

Electrochemical methods can be utilized to effectively separate actinide and lanthanide species from complex mixtures. This is based on the general description of electrochemical control of precipitation or dissolution. The selective dissolution or precipitation of a chemical species is based on the thermodynamic potential dependent oxidation/reduction of the chemical species in the solid. Each chemical species has unique electrochemical properties largely based on physical properties such as ionization and chemical potential, which determine the potential for dissolution.

The same thermodynamic properties identified for species dissolution from solids can be used in the deposition of these species at electrochemically controlled interfaces. Evaluating the oxidation/reduction properties and determining the reaction

mechanism of each species in solution is the key to effective separations and optimization of such processes. Thus, it may be possible to selectively separate individual species electrochemically from a mixture.

RESEARCH OBJECTIVES AND METHODS

The objective of this project is to use electrochemical techniques to develop a thermodynamic understanding of actinide and lanthanide species in aqueous solution and use this data to effectively separate species with very similar chemical properties. In consultation with our DOE collaborator, electrochemical methods and materials will be evaluated and used to exploit the thermodynamic differences between similar chemical species enhancing our ability to selectively target and sequester individual species from mixtures. The project can be divided into three distinct phases that can be defined by one-year intervals.

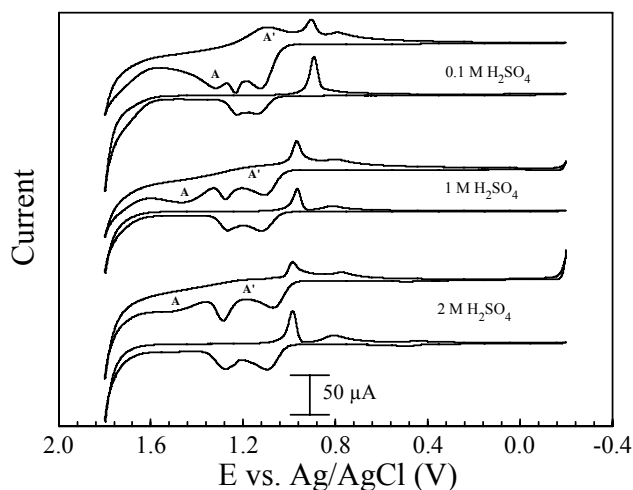
Phase 1: The thermodynamic oxidation/reduction properties of actinides and lanthanides will be examined using electrochemical methods. How the oxidation/reduction of actinides and lanthanides change after complex formation will also be examined.

Phase 2: The thermodynamics studies in phase I will be expanded to include the potential mediated adsorption properties of lanthanide and actinide species at Hg and Au/Hg electrodes. It is expected that the thermodynamics of adsorption will be markedly different than the oxidation/reduction.

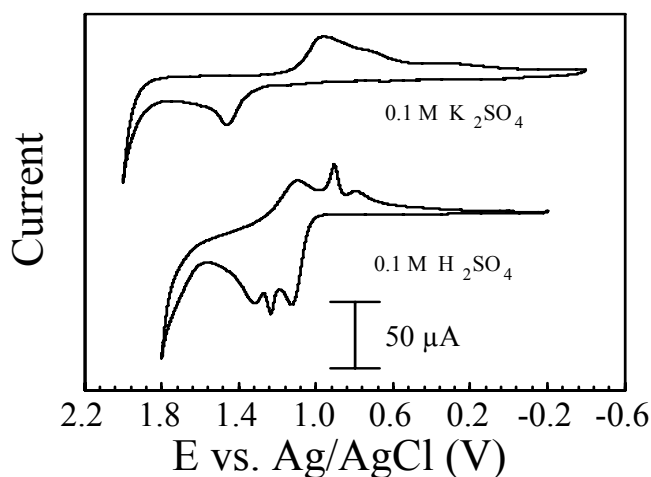
Phase 3: The use of conductive polymer membranes for the uptake and expulsion of complexed and uncomplexed actinide and lanthanide species will be examined. The uptake and selective adsorption and separation of individual actinide and lanthanide species including the isolation of Cm from Am will be examined using conductive polymer/metal composite membranes containing bound chelates. The potential mediated separation of single chemical species within a mixture will be the focus.

The following were specific goals for this year:

- To develop a fundamental understanding of the thermodynamic properties of actinide and lanthanide species such as Cm, Am, Ce, Nd, Eu, Sm prior to complex formation.
- To examine how chelation influences the thermodynamic properties of waste form species.
- To use systematic studies to distinguish the thermodynamic signatures and ability to shift thermodynamic potentials using chelation to enhance separation properties.



Influence of acid concentration on the redox properties of 6mM $\text{Ce}(\text{NO}_3)_3$. The redox couple $\text{Ce}^{3+}/\text{Ce}^{4+}$ are labeled using A and A'. The background in the supporting electrolyte is presented below the cyclic voltammetry for the solution containing Ce. Working electrode was an Au disk.



Influence of acid concentration on the redox properties of 6mM $\text{Ce}(\text{NO}_3)_3$ with constant ionic strength $\mu = 0.3 \text{ M}$. Working electrode was an Au disk.

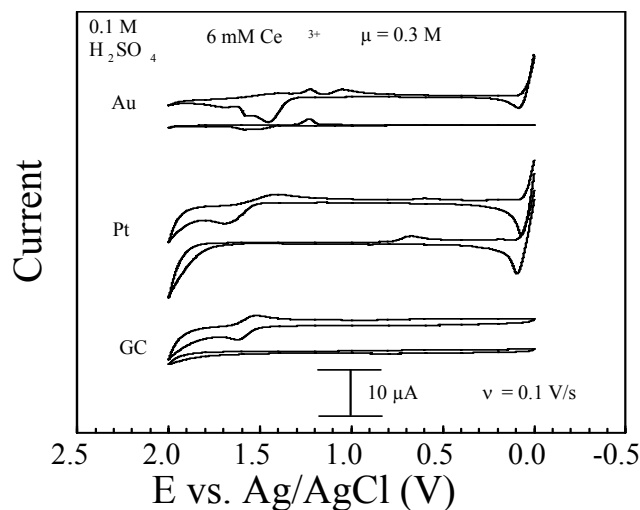
The effect of Ce oxidation and reduction was also examined with respect to the ionic strength of the solution. In these studies the concentration of K_2SO_4 was used to replace the H_2SO_4 supporting electrolyte solutions. The goal of this study was to distinguish the role of ionic strength versus pH for the Ce electrochemistry. The results are presented in the figure (above left) for a system with an ionic strength of $\mu = 0.3 \text{ M}$. The data suggests that acidity is the key variable in the system with higher resolution and lower splitting of the $\text{Ce}^{3+}/\text{Ce}^{4+}$ redox couple.

The voltammetric response was also obtained at Au, Pt and glassy carbon electrodes. Resolution for each electrode is quite different. Peak splitting for each electrode provides information regarding the reversibility of the reaction. The figure (above right) shows the voltammetric response for the three electrodes under optimum acid conditions. Pt and glassy carbon electrodes display higher resolution in comparison to Au due to the lack of background signal in supporting electrolyte. In addition, the peak splitting for Pt and glassy carbon is sufficiently small in comparison to Au indicating the reaction is more reversible at these two electrodes. Glassy carbon has the smallest peak splitting indicating the electrode has the best thermodynamic reversibility.

Significantly different results are obtained for acetate buffer solutions at $\text{pH} = 7.5$. The data at this pH is characterized by a loss of electrochemical resolution for the Au and Pt electrodes. The redox properties of Ce at glassy carbon is still visible with lower resolution and larger peak splitting. In each case the reversibility and resolution of the redox couple is diminished.

ACADEMIC YEAR HIGHLIGHTS

- ♦ "The Electrochemical Characterization of Ce at Au, Pt and Glassy Carbon Electrodes: Influence of pH and Ionic Strength," by S. Elkouz, K. Czerwinski, and D.W. Hatchett, manuscript in preparation (2005).



Influence of working electrode composition on the redox prop-

FUTURE WORK

Future work will focus on identifying the optimized solution parameters for other species of interest including Sm, Eu, and Nd. The redox properties of these species will require that a systematic treatment be employed to determine the stability of the redox species as a function of solution pH, species concentration, and ionic strength. The task will be hindered by the lack of published data on the given systems. The goal is to understand the redox properties such that they can be optimized and manipulated to provide an effective method to differentiate individual species in complex mixtures.

In the immediate future the complexation and speciation of Ce and Sm will be examined. How the oxidation/reduction of actinides and lanthanides change after complex formation will be examined. The goal is to shift the thermodynamic potentials to ensure that species can be distinguished and separated from complex mixtures. A thorough understanding of parameters such as ionic strength and pH are critical in complex formation and will be the basis for these studies.

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Task 26

Fundamental Chemistry of U and Pu in the TBP-Dodecane-Nitric Acid System

K. Czerwinski and B. Bennett

BACKGROUND

The extraction of tetravalent Pu in nitric acid solution by tributylphosphate (TBP) is well known and has been the basis of Pu purification for a number of decades. The extraction is based on the formation of an organic phase neutral complexes such as $\text{Pu}(\text{NO}_3)_4 \cdot 2\text{TBP}$. Upon reduction, the trivalent Pu species is back extracted into an aqueous phase. However, the data needed for detailed modeling of Pu extraction is not available for all conditions of concern to the AFCI. Based on the direction from Dr. George Vandegrift of Argonne National Laboratory, this proposal was developed to obtain the necessary data for Pu extraction modeling.

Understanding the role of nitrate in Pu speciation is important for determining the necessary data for Pu extraction modeling. Data indicates the dinitrate complex of Pu is strong and may account for difficulties in modeling Pu extraction under some nitrate conditions. The formation of hydrolysis products may also form an extractable species that will need to be included in modeling.

In the UREX process, acetohydroxamic acid (AHA) is expected to be used. The interaction of AHA with tetravalent Pu decreases extraction into the organic phase by either complex formation or reduction of Pu to the trivalent state. For the separation of Pu in a solvent extraction system using acetohydroxamic acid, it is necessary to determine the complexation kinetics and thermodynamics.

In addition, since Pu is a redox sensitive element, the change in speciation due to oxidation-reduction reactions upon complexation needs to be evaluated. This project experimentally evaluates the fundamental speciation of Pu and U in the TBP-dodecane-nitric acid system, with the main emphasis on nitrate speciation and subsequent third phase formation at high nitric and metal ion conditions. Experiments on the AHA systems are conducted in collaboration with input from the AFCI separations group.

RESEARCH OBJECTIVES AND METHODS

The research objectives of this project are as follows:

- To determine the influence of nitrate on the speciation of U and Pu in the TBP-dodecane-nitric acid system. The aqueous and organic speciation of U and Pu are examined as a function of the nitric acid concentration, nitrate concentration (by the addition of NaNO_3), actinide ion concentration, temperature, and time.
- To determine the speciation of U and Pu with AHA in the presence and absence of TBP-dodecane organic phase. The aqueous and organic speciation of U and Pu are evaluated

as a function of AHA concentration, metal ion concentration, metal ion redox state, pH, and temperature. Experiments will initially examine the aqueous phase then examine the two phase system.

- To incorporate thermodynamic and kinetic data into existing modeling codes.

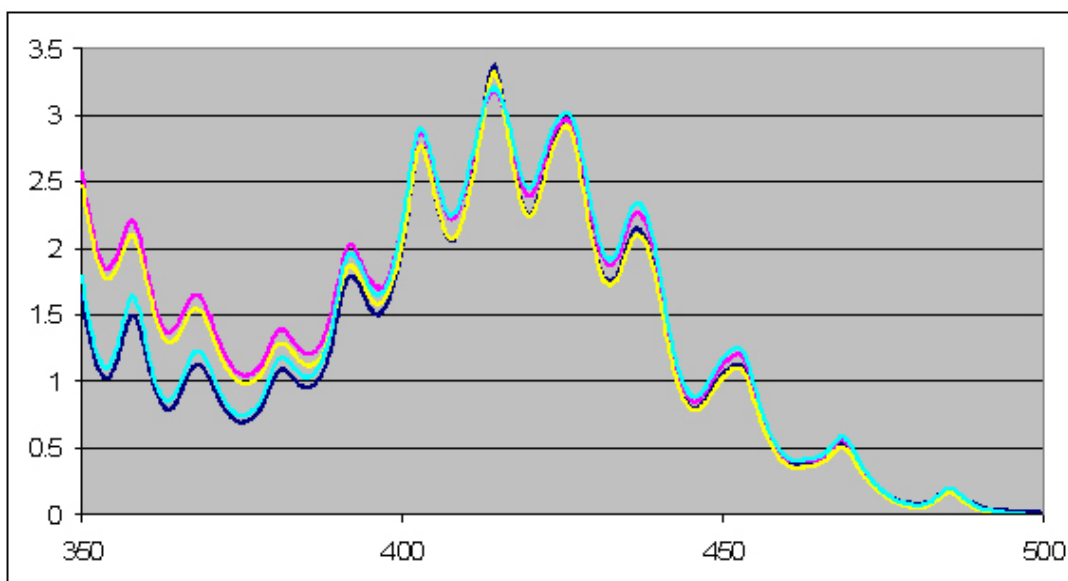
The following experimental techniques are used in the evaluation of U and Pu speciation: UV-Visible spectroscopy, Time resolved laser fluorescence spectroscopy, NMR spectroscopy, IR spectroscopy, Raman spectroscopy, Titrations, ICP-MS, ICP-AES, XAFS, and Electrochemical.

Initial experiments are performed with UO_2^{2+} . The initial results obtained with UO_2^{2+} are the basis for further experiments with Pu. In extraction experiments, the aqueous and organic phases are equal volumes and range from 0.5 mL to 5.0 mL. The actinide ion concentration varies from mmol/L to the mmol/L range. Nitrate concentration varies from the concentration due to nitric acid by the addition of NaNO_3 . The nitric acid concentration varies from 14 M to the pH range in experiments with AHA. The temperature varies from 20 °C to 80 °C. The results will be used to determine Gibbs free energy.

RESEARCH ACCOMPLISHMENTS

Studies were performed on the extraction of uranium from nitric acid into 30 % TBP in dodecane as a function of nitrate concentration. Stock solutions of uranyl nitrate were prepared at constant nitric acid concentration by dissolution of known quantities of $\text{UO}_2(\text{NO}_3)_2 \cdot 6\text{H}_2\text{O}$ (Merck) in nitric acid solutions. Organic extraction phases were prepared using 30 vol. % tributyl phosphate (Aldrich 97 %) with n-dodecane (Prolabo). Nitrate concentration was adjusted by the addition of concentrated LiNO_3 . Equal volumes of 5 mL organic and aqueous phases were contacted and vigorously mixed for 5 minutes then allowed to mix on a shaker table for 5 hours. After centrifuging, samples of each phase were drawn off and spectra taken using a Cary UV-visible spectrometer with precision quartz cuvettes (1 cm path length) measured against a deionized water reference cell. Four sets of spectra were collected for each sample and the average used in analysis performed with Microsoft Excel™ software.

Improvement of the extraction methods was undertaken. The volume of aqueous and organic phase used was reduced to 1.6 mL. Spectroscopy is still possible with these volumes and waste volume is minimized. The determination of nitrate concentration in the organic phase has been measured by ion specific electrode and ion chromatography. For the ion specific electrode the system is found to be highly dependent upon the total acid concentration. Up to 5 % drift with same standards and 12



Comparison of quartz to PMMA cuvettes: Blue and yellow are quartz; teal and fuschia are PMMA.

% drift with variations in total acid concentration was observed. Nitrate ion chromatography shows accuracy of 5% and no acid effects are observed. UV-visible spectra were collected for a number of TBP/dodecane extractions of uranium (see figure above).

A number of different nitrate concentrations were examined. The following conditions were found for third phase formation as measured at 18°C:

- For 1 M U, need $[\text{NO}_3]_{\text{tot}} \geq 10.2 \text{ M}$, $[\text{HNO}_3] > 5 \text{ M}$
- For 0.5 M U, need $[\text{NO}_3]_{\text{tot}} > 11 \text{ M}$, $[\text{HNO}_3] > 7 \text{ M}$,
- For 10 M HNO_3 , no nitrate need $[\text{U}] \sim 0.57 \text{ M}$
- For 12 M HNO_3 , no nitrate need $[\text{U}] \sim 0.185 \text{ M}$
- For 13 M HNO_3 , no nitrate need $[\text{U}] \sim 0.08 \text{ M}$
- For 14 M HNO_3 , no nitrate need $[\text{U}] \sim 0.022 \text{ M}$
- For 14 M $[\text{NO}_3]_{\text{tot}}$ and 10 M $[\text{HNO}_3]$, need $[\text{U}] \sim 0.062 \text{ M}$
- For 12 M $[\text{NO}_3]_{\text{tot}}$ and 8 M $[\text{HNO}_3]$, need $[\text{U}] \sim 0.42 \text{ M}$

The results on nitrate organic concentration at 12 M HNO_3 , 12 M total nitrate, and 14 M HNO_3 show that the bulk of the nitrate remains in the aqueous phase. The total nitrate extracted appears independent of initial uranium, nitrate, and nitric acid concentrations.

When the organic phase splits, the heavy phases has about 2 –

2.5 M $[\text{NO}_3]$ and the light phases have about 1-1.2 M $[\text{NO}_3]$. Single phases have about 1.3-1.5 M $[\text{NO}_3]$, similar to the light 2nd phase. High $[\text{NO}_3^-]$ is found to encourages complete extraction of U into a heavy phase. Kinetic effects on third phase formation were observed.

Work also focused on 3rd phase formation studies with the uranyl system. which happens with the organic phase spontaneously splits into a light and a heavy phase. This phenomenon occurs when the uranium and nitric acid concentrations exceed a certain threshold. Current theories include that the third phase forms gradually in small reverse micelles when uranyl and nitric acid reach a certain limiting organic concentration (LOC) that makes it thermodynamically favorable to separate and form a different structure. This is analogous to the critical micelle concentration (cmc) in surfactant micelle formation. The third phase formation is quite dependent on temperature. There has been some work indicating that the UV-visible spectrum changes at certain wavelengths as the system approaches third phase, indicating a variation in the uranyl electronic structure as this third phase begins to form.

Furthermore, the role of nitrate vs. nitric acid in third phase formation was evaluated. To this end, hundreds of samples were generated over a spectrum of concentrations for U, LiNO_3 , and HNO_3 .

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Task 27

Reactor Physics Studies for the AFCI Reactor-Accelerator Coupling Experiments (RACE) Project

D. Beller

BACKGROUND

In the RACE Project of the U.S. Advanced Fuel Cycle Initiative (AFCI), a series of accelerator-driven subcritical systems (ADSS) experiments will be conducted at the Idaho State University's Idaho Accelerator Center (ISU-IAC), at the University of Texas (UT) at Austin, and at the Texas A&M University. In these experiments, we will use electron accelerators to induce bremsstrahlung photon-neutron reactions in heavy-metal targets. A beam power of 1 kW will produce a neutron source of 10^{12} n/s, which will then initiate fission reactions in the subcritical systems.

These systems will include a compact, transportable assembly at ISU and TRIGA reactors at UT-Austin and Texas A&M. A variety of fuel and assembly geometries will be studied: at ISU we will use 150 flat plates of 20%-enriched uranium-aluminum alloy plated with aluminum; at UT-Austin a 20%-enriched UZr-H fuel will be used; and at Texas A&M a 70%-enriched UZr-H "FLIP" fuel will be used as well as a used core of 20%-enriched UZr-H fuel. The use of compact accelerators and a small target will allow the placement of the target in various positions in or adjacent to these subcritical assemblies to "map" the coupling of driven neutron sources; measuring core coupling and mapping adjoint flux.

The RACE Project is an important intermediate step between

the recent European program MUSE and a future near full-scale demo like the TRADE project. For MUSE, which was conducted by the CEA at Cadarache, France, the driving neutron source was produced by D-D or D-T reactions which produce a mono-energetic source of 2.45 or 14.1 MeV and a maximum strength of $\sim 10^{10}$ n/s. For TRADE (ENEA, Casaccia, Italy), the source will be provided by spallation from a proton cyclotron, with an anisotropic source up to ~ 140 MeV and $\sim 10^{15}$ n/s. For design of full scale ADSS, a complete knowledge of the effects of the driving neutron source is essential. This will ultimately require spectral, temporal, directional, and intensity fidelity in prototype experiments. In the absence of this fidelity, simulated sources should match some of the characteristics of projected driving sources to build confidence in predicting performance of these systems, and codes and methods must be validated.

The RACE Project will provide experience in a higher energy range (above 14.1 MeV up to 40 MeV) and with a stronger and more isotropic source than the MUSE experiments. In addition, RACE will provide valuable information on thermal feedback effects in the TRIGA reactors. Finally, and possibly most important, because of the mobility of compact electron linacs connected to compact targets by easily fabricated vacuum tubes, RACE will permit source importance mapping and adjoint flux studies because of the ability to relocate the target between experiments. This combination of attributes of the



UNLV students Evgeny Stankovskiy (far left) and Timothy Beller (kneeling far right) with other participants in the RACE and ECATS projects after the joint RACE-ECATS.

RACE Project will provide highly valuable information in advance of the TRADE program.

RESEARCH OBJECTIVES AND METHODS

The specific research objective of this three-year project is to design and conduct an accelerator driven experiment at one of the Texas universities. This experiment will help demonstrate in the U.S. the ability to design, compute, and conduct ADSS experiments; and to predict and measure source importance, coupling efficiency, sub-critical reactor kinetics and source-driven transients. In addition, both steady state and transient ADSS benchmarks will be created for the nuclear community to develop and test new computational codes and methods, and the importance of a driving neutron source in various regions of different sub-critical assemblies will be mapped. Experiments will be conducted and compared to calculations with radiation transport and thermal-hydraulics codes such as MCNPX and RELAP.

RESEARCH ACCOMPLISHMENTS

Reactor Physics Studies

The Radiation Safety Information Computational Center (RSICC) at Oak Ridge National Laboratory granted Evgeny Stankovskiy access to a set of export-controlled codes and databases for reactor physics studies. Modeling with MCNPX was initiated in support of subcritical experiments at the Idaho Accelerator Center and of target design studies for Texas RACE. Electron beam/target interactions were studied for maximizing and characterizing photoneutron production from high-energy electrons. The newest beta test version of the MCNPX radiation transport code was acquired, installed, and used.

Preparations for Experiments

Collaborations began with Texas RACE Project participants to develop a plan to conduct an accelerator-driven subcritical experiment at UT-Austin or Texas A&M University. Principle Investigators and graduate students from the Texas universities visited UNLV in December and January to discuss preparations for experiments and MCNP modeling of the RACE Project configurations at ISU, UT, and TAMU.

ACADEMIC YEAR HIGHLIGHTS

- ◆ A large European ADS program has joined the RACE Project to participate in experiments at UT-Austin and Texas A&M.
- ◆ “Overview of the AFCI Reactor-Accelerator Coupling Experiments (RACE) Project,” D. Beller, *Transactions of American Nuclear Society*, 90, Pittsburgh, PA, June 14-17, 2004.
- ◆ “Initial Results from the AFCI Reactor-Accelerator Coupling Experiments (RACE) Project,” D. Beller, A. Hunt, J. Bennion, M. Garfield, K. Folkman, and M. Reda, *Transactions of American Nuclear Society*, 91, 446-447, Washington, DC, Nov. 14-18, 2004.
- ◆ “AFCI Reactor-Accelerator Coupling Experiments Program,” D. E. Beller, oral presentation, AFCI Semi-annual Technical Program Review, Salt Lake City, Utah, September 13, 2004.
- ◆ “Initial Results from the AFCI Reactor-Accelerator Coupling Experiments (RACE) Project,” D. Beller, A. Hunt, M. Reda, and J. Bennion, poster presentation, to be published by OECD-NEA in the *Proceedings of the Eighth Information Exchange Meeting on Actinide and Fission Product Partitioning & Transmutation*, 9-11 November 2004, Las Vegas, Nevada.
- ◆ “Overview of the AFCI Reactor-Accelerator Coupling Experiments (RACE) Project,” D. Beller, oral presentation, to be published by OECD-NEA in the *Proceedings of the Eighth Information Exchange Meeting on Actinide and Fission Product Partitioning & Transmutation*, 9-11 November 2004, Las Vegas, Nevada.
- ◆ “Overview of the AFCI Reactor-Accelerator Coupling Experiments (RACE) Project,” D. Beller, GenIV/AFCI Nuclear Data Working Group and AFCI Physics Working Group Meetings, Las Vegas, Nevada, January 28, 2005.

FUTURE WORK

During the summer of 2005, an ADSS experiment is planned using an ISU-supplied 20- or 25-MeV electron linac accelerator and the TRIGA reactor at UT-Austin. This experiment will be planned in conjunction with participants from EUROTRANS ECATS. During the experiment we will measure actual fission energy production induced by accelerator-generated neutrons.

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Transmutation Research Program Infrastructure Augmentation User Facility Highlights

Transmission Electron Microscopy Laboratory

Modern technology pushes the limits of materials in many ways: the development of radiation-resistant structural materials, the development of lead-bismuth eutectic resistant coatings, the understanding of the human body at the micro-cellular level, and even the development of nanometer-scale machines and systems. The key to the development of all these fields is the ability to examine and investigate materials at the atomic level.



Electron microscopy is the primary method to determine structure and chemistry of structural features such as interfaces or dislocations.

The Transmission Electron Microscopy Laboratory provides researches at UNLV with the ability to characterize ceramics, metals, and biological materials at resolutions



down to atomic scale, with a resolution of 2 Ångström (0.2 nm). Magnifications of typically 1,000,000 times or higher can be achieved. The system allows qualitative chemical analysis energy dispersive X-ray spectroscopy (EDS), parallel energy loss spectroscopy (PEELS), and energy-filtered electron microscopy (EFTEM). In support of many of the Advanced Fuel Cycle Initiative and related programs, the system at UNLV has been licensed to allow the imaging of radioactive samples, allowing the use of this state-of-the-art technique to investigate the materials properties of nuclear fuel and radiation-damaged structural components.

Electron Microscopy Sample Preparation Laboratory

Sample preparation is the critical step in any microscopy application. This is particularly true for Transmission Electron Microscopy, where the sample to be investigated needs to be prepared in a section that is much less than 1 micron (1 μm) thick. The Electron Microscopy Sample Preparation Laboratory provides researchers with access



Multi-Preparation System



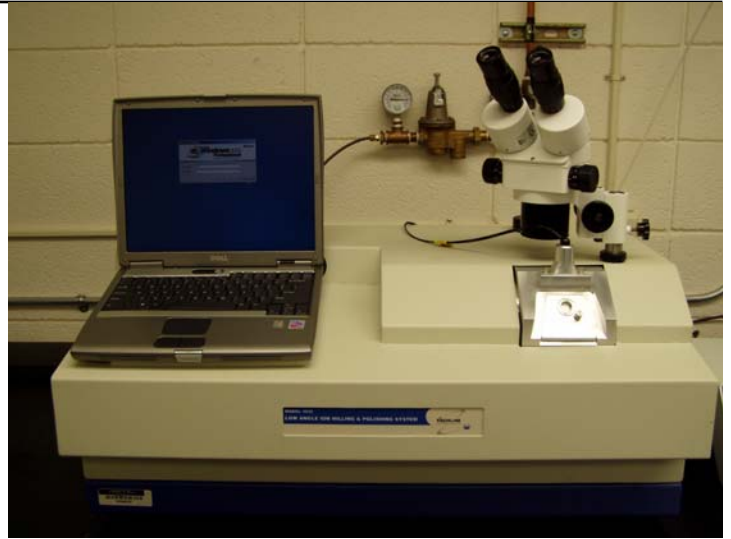
Tuned-Piezo Ultrasonic Cutter

to the state-of-the-art in sample preparation technology in order to produce high quality TEM and SEM specimens for a variety of materials constitution, including ultramicrotomes, ultrasonic cutters, mechanical dimplers, electro-chemical polishers, and a low-angle ion mill. These systems are augmented by the traditional sample preparation tools, such as grinder/polishers, sample saws, and optical microscopes, to allow researchers to fine-tune their samples regardless of the sample material.

Transmutation Research Program Infrastructure Augmentation User Facility Highlights



Dimpler



Low Angle Ion Mill

Electron Microscopy Sample Preparation Laboratory for Radioactive Samples

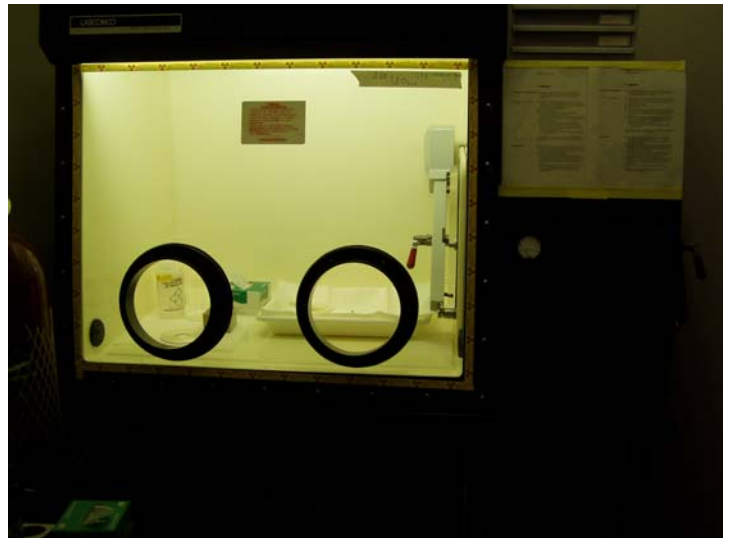
One of the unique capabilities of the microscopy facilities at UNLV is that researchers are allowed to image radioactive materials directly on the systems. In support of this capability, the UNLV TRP commissioned the installation of additional sample preparation equipment dedicated to the preparation of radioactive samples. This additional capability is fully contained within a radiation laboratory, and is supported by an internally recycled water/waste system, allowing researchers to cut, grind, and polish radioactive samples safely without risking the contamination of the general-use sample preparation facility.



Ultra-Microtome



Multi-Preparation System, High-end Polisher/Grinder, Low Speed Saw, Vacuum Impregnation System



Alpha-Glove Box for Sample Preparation

Transmutation Research Program Infrastructure Augmentation User Facility Highlights

High Temperature Materials Experimental Facility

The High Temperature Materials Experimental Facility is designed to support materials investigations at high temperatures, and in particular experiments utilizing molten Lead Bismuth Eutectic (LBE). The layout of the facility is shown in the figure to the right.

At the back wall on the left is a stainless steel 5' perchloric acid hood with wash-down and independent ventilation. This hood is very well suited for housing high temperature apparatuses.

Next to the hood is a sink/eyewash, and acid cabinet with a top polyethylene work surface. This area may be used for "wet" work.

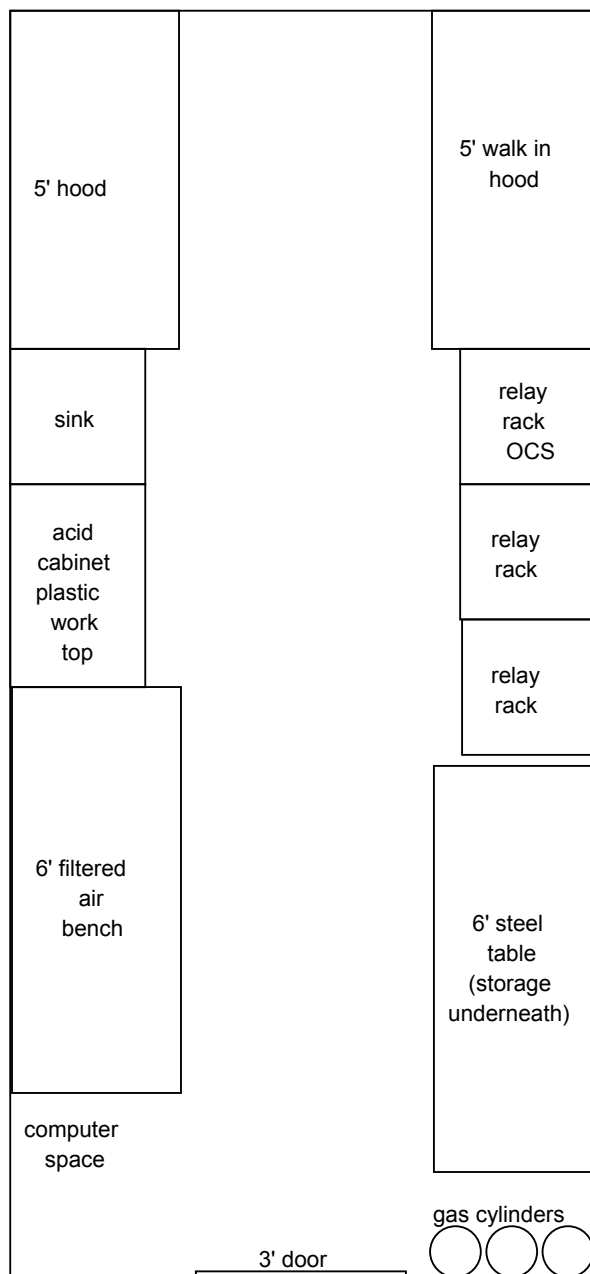
Next to the acid cabinet is a HEPA filtered work bench to provide clean and safe work environments if dangerous particulates (e.g. LBE) might be generated.

Next to the door are the computer facilities. Gas storage is on the right from the door. Next is a stainless steel table, where a tube furnace for gas phase studies will be located. At the far end is space for equipment racks and optionally a walk in hood for additional experiments.

The left side view (shown below right) shows the perchloric acid hood, acid cabinet, and filtered hood. The filtered hood is a commercially available biological safety hood.

The view from the back (below) shows the steel table, gas cylinder storage area, filtered hood, and acid cabinet.

In summer of 2005, safety equipment and an Oxygen Control System will be installed and gas phase experiments are expected to begin.



Laboratory layout



View from the back wall



View from door

Transmutation Research Program Infrastructure Augmentation Faculty Highlights

Yitung Chen is an Associate Professor of the Department of Mechanical Engineering and Associate Director of the Nevada Center for Advanced Computational Methods (NCACM) at the University of Nevada Las Vegas. He received his Ph.D. in Mechanical Engineering from the University of Utah, Salt Lake City, UT in 1991. He also has a minor in Nuclear Engineering. His area of expertise is computational fluid dynamics, numerical heat and mass transfer, lattice Boltzman method, perturbation method, high performance computing, compressible flow simulation, atmospheric and environmental modeling, groundwater flow, thermal system design, renewable energy, and bioengineering. He also has a strong background in organic chemistry, biochemistry, polymer chemistry, and physical chemistry. Currently, he serves as Principal Investigator for two research projects for the Transmutation Research Program. These include Task 21 "Theoretical Modeling of Protective Oxide Layer Growth in Non-isothermal Lead-Alloys Coolant Systems" and Task 24 "Development of Integrated Process Simulation System Model for Spent Fuel Treatment Facility (SFTF) Design."



Yitung Chen

Thomas Hartmann joined the Harry Reid Center for Environmental Studies at UNLV as Research Scientist in October 2004. He received his M.S. degree (1991) as well as his doctoral degree in Mineralogy (1995) at the University of Heidelberg, Germany. In his thesis he investigated the ternary Pd-Rh-Te metal system in the vitrification process of radioactive high-level liquid waste concentrates deploying liquid-feed ceramic melter technology. In 1995 he became a staff member and team leader at the Research Center at Karlsruhe (FZK), Germany, and collaborated with the Siemens/KWU Company, coordinating and performing research at the Thermal Waste Recycling pilot plant of Siemens/KWU. In 1997 he joined Los Alamos National Laboratory as a postdoctoral fellow performing experimental work on irradiation-induced structural damage in possible ceramic host phases for actinides. In 1999 he became technical staff and principal investigator for *NTISV in-situ* vitrification and in 2000 principal investigator for the LANL actinide chemistry program to support the DOE WIPP project at Carlsbad, NM.



Thomas Hartmann

Dr. Hartmann's area of expertise is solid phase analysis and X-ray crystallography, using X-ray and neutron diffraction, Rietveld structure- and least-square refinement, optical microscopy, electron microscopy (SEM, EPMA, TEM), thermal analysis (DTA, TGA, DSC), X-ray fluorescence, and Rutherford backscattering spectroscopy (RBS). He is an expert in waste vitrification, repository science, and radiolysis. Dr. Hartmann's research at UNLV HRC is focusing on the development, synthesis and performance of inert matrix nuclear fuel candidates. Dr. Hartmann is the director of the new Structure and Solid Phase Analysis (S-SPA) group at the HRC.



Jian Ma

Jian Ma joined the Mechanical Engineering Department of UNLV as an Assistant Research Professor in May 2005. He received his Ph.D. in Mechanical and Production Engineering School from Nanyang Technological University, Singapore in 2004. His area of expertise is fluid dynamics. He has worked on applications in various aspects of molten metal thermodynamics, sensing system for oxygen concentration, non-intrusive fluid diagnosis, plasma spray technology for ceramic coating, heat and mass transfer as well as the wind engineering. Within the Transmutation Research Program, Dr. Ma is the director of the Target Complex 1 (TC-1) and Lead Calibration Stand. These molten metal facilities are necessary to extend research in experimental thermal hydraulics, oxygen control against corrosion, high temperature heat exchange, and oxygen sensor development.

UNLV TRP EVENTS

June 4, 2004

The Board of Regents approve the Materials and Nuclear Engineering M.S. Program proposal.

September 2-3, 2004

Three faculty members participate in the Modular Helium Reactor Deep Burn workshop sponsored by General Atomics in La Jolla, CA.

September 15, 2004

John C. Browne (former LANL Director) presents a lecture at UNLV "Material Controls and Accountability, Nunn-Luger, and International Export Control."

October 1-3, 2004

Transmutation poster and literature displayed at the Pahump Fall Festival.

October 4, 2004

Thomas Hartmann, a mineralogist with past experience at LANL and FZK (Germany), is hired by the TRP as a research professor in support of the Actinide Chemistry Group at UNLV.

October 4 and 6, 2004

UNLV TRP hosts Glenn Knoll (University of Michigan) for a two-part lecture at UNLV "Nuclear Radiation Detection Fundamentals."

November 8, 2004

UNLV TRP hosts a tour of Yucca Mountain for participants at the OECD/NEA Partitioning and Transmutation meeting.

November 9-11, 2004

UNLV TRP hosts the Eighth Annual OECD/NEA Actinide and Fission Product Partitioning and Transmutation Information Exchange Meeting. 120 people from 22 countries attend the meeting.

November 9, 2004

Remodeling of the Actinide Chemistry Laboratory was completed and commissioned with representatives from the DOE AFCI and France.

November 16, 2004

Installation is completed on a UNLV TRP-sponsored Inductively Coupled Plasma Atomic Emissions Spectrometer (ICP-AES) at UNLV.

October 15, 2004

ANS UNLV Student Section holds elections. Suresh Sadineni elected as President.

December 4-18, 2004

Six Russian scientists visit UNLV to continue installation of TC-1 lead-bismuth eutectic loop.

December 8, 2004

UNLV TRP Director meets with DOE NE Director William Magwood and Deputy Director Shane Johnson in Germantown, MD.

December 10, 2004

E. Chris Hagen (Bechtel/Nevada) gives an ANS seminar at UNLV "An Overview of the Dense Plasma Focus Project at the Nevada Test Site."

December 13, 2004

Sen. Pete Domenici (R-NM) gives a lecture and book signing at the Atomic Testing Museum, Las Vegas, NV.

January 26, 2005

UNLV hosts a Deep Burn Work Package Development meeting. Nine work packages are drafted.

January 27-28, 2005

UNLV hosts the joint AFCI/Gen IV Nuclear Data Working Group and the AFCI Physics Working Group meetings.

January 11, 2005

James Tulenko (ANS President) presents a seminar at the ANS Nevada Section "Energy, Environment and the Economy."

February 7, 2005

Denis Beller is appointed as coordinator of the Nuclear Engineering M.S. program at UNLV.

March 4, 2005

Lee Dodds (University of Tennessee) gives an ANS seminar at UNLV "Recent Developments in Nuclear Power."

March 25, 2005

Twenty UNLV students tour the Palo Verde Nuclear Generating Station (Wintersberg, AZ), the largest nuclear electric generating site in the U.S.

April 15-17, 2005

Thirteen UNLV TRP students present papers at the ANS Student Conference in Columbus, Ohio. UNLV TRP students receive three session awards.

April 28, 2005

Bernie Copsey (Framatome, ANP) presents a seminar at UNLV "The European Pressurized Reactor and Framatome's High Temperature Reactor Design."

May 20, 2005

Scott Palmtag (Studsvik Scandpower) present a seminar at UNLV "Reactor Physics Applications for Commercial Nuclear Reactors."

Transmutation Research Program Financial Statement

Program Administration	FY01	FY02	FY03	FY04	TOTAL
Program Support					
Labor	\$187,305	\$348,324	\$536,041	\$441,349	\$1,513,019
Other Costs (e.g. travel, services, supplies)	\$121,779	\$72,336	\$114,486	\$105,000	\$413,601
LANL Subcontract	\$150,000	\$162,500	\$0	\$0	\$312,500
Infrastructure Augmentation: New Hires	\$112,692	\$240,648	\$394,000	\$380,000	\$1,127,340
Infrastructure Augmentation: Facilities	\$1,492,446	\$799,837	\$804,077	\$605,922	\$3,702,282
Infrastructure Augmentation: Academic	\$0	\$0	\$0	\$181,200	\$181,200
International Collaboration	\$144,973	\$377,175	\$258,250	\$121,700	\$902,098

Student Research Task by Task							
	FY01	FY02	FY03	FY04	TOTAL		FY04
Task 1	\$97,379	\$185,495	\$141,417	\$0	\$424,291	Task 17	\$165,253
Task 2	\$127,146	\$195,148	\$161,147	\$0	\$483,441	Task 18	\$149,704
Task 3	\$98,896	\$285,346	\$192,321	\$0	\$576,563	Task 19	\$140,865
Task 4	\$108,615	\$179,270	\$144,794	\$0	\$432,679	Task 20	\$103,587
Task 5	\$40,655	\$142,081	\$89,214	\$3,044	\$274,994	Task 21	\$106,290
Task 6	\$58,952	\$219,403	\$90,863	\$0	\$369,218	Task 22	\$56,921
Task 7	\$55,565	\$201,791	\$160,324	\$32,283	\$449,963	Task 23	\$79,941
Task 8	\$57,700	\$206,215	\$86,441	-\$266	\$350,090	Task 24	\$124,228
Task 9	\$21,609	\$109,376	\$71,167	\$18,850	\$221,002	Task 25	\$91,545
Task 10	\$57,175	\$112,610	\$74,147	\$0	\$243,932	Task 26	\$135,776
Task 11	\$41,308	\$68,815	\$69,110	\$23,711	\$202,944	Task 27	\$79,950
Task 12	\$25,805	\$146,974	\$81,792	\$27,404	\$281,975		
Task 13	\$0	\$146,048	\$172,502	\$105,697	\$424,247		
Task 14	\$0	\$120,438	\$107,073	\$82,491	\$310,002		
Task 15	\$0	\$74,050	\$64,833	\$63,389	\$202,272		
Task 16	\$0	\$106,120	\$46,001	\$74,166	\$226,287		
Totals	\$790,805	\$2,499,180	\$1,753,146				\$1,664,829

Infrastructure Facilities Augmentation

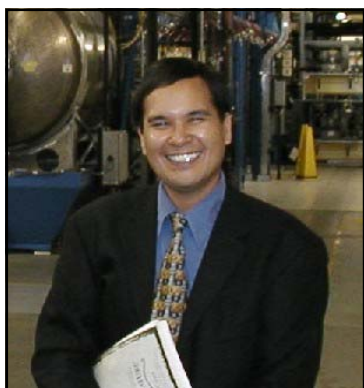
	FY01	FY02	FY03	FY04	Total
Electron Microanalysis and Imaging Laboratory	\$42,313	\$63,000	\$63,000	\$63,000	\$231,313
Materials Performance Laboratory	\$150,133	\$77,360	\$0	\$18,300	\$245,793
Transmission Electron Microscope	\$1,300,000	\$159,369	\$321,582	\$150,000	\$1,930,951
ICP – Atomic Emission Spectrometer	\$0	\$100,163	\$0	\$0	\$100,163
Lead-Bismuth Eutectic Facilities	\$0	\$234,198	\$146,995	\$200,000	\$581,193
Machining System and Equipment	\$0	\$72,619	\$22,500	\$822	\$95,941
Flow Visualization System (Task 2)	\$0	\$22,207	\$0	\$0	\$22,207
Pyrolizer, Baths, and Controller (Task 15)	\$0	\$20,921	\$0	\$0	\$20,921
Prof. B.J. Das Startup Package Equipment	\$0	\$50,000	\$50,000	\$0	\$100,000
Actinide Chemistry Laboratory	\$0	\$0	\$200,000	\$123,800	\$323,800
Oxygen in LBE Control System	\$0	\$0	\$0	\$50,000	\$50,000
Totals	\$1,492,446	\$799,837	\$804,077	\$605,922	\$3,702,282

International Collaboration

Khlopin Radium Institute Contracts	\$113,050	\$229,500	\$127,000	\$0	\$469,550
International Science and Technology Center		\$87,500	\$98,250	\$51,700	\$237,450
International Collaboration Program Coordination	\$31,923	\$60,175	\$33,000	\$70,000	\$195,098
Totals	\$144,973	\$377,175	\$258,250	\$121,700	\$902,098

Photo Gallery

Transmutation Research Program Administration



**Director,
Anthony E. Hechanova
(HRC)**



**Finance Director,
Patricia Rugeiro
(HRC)**



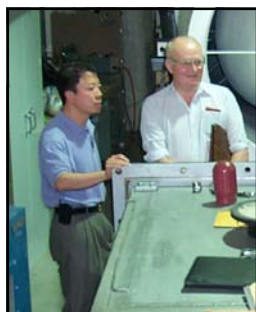
**Deputy Director
Gary S. Cerefice
(HRC)**



**Deputy Director
of Engineering
William G. Culbreth**



**Deputy Director
College of Science
Malcolm F. Nicol**



**International Programs
Coordinator
Ning Li (LANL)**

Ning Li and Evgeny Yefimov (former IPPE Laboratory Head who passed away Dec. 29, 2003)) with Russian-built loop at UNLV.



**International Programs
Adviser
Thomas Ward**

Thomas Ward and Khlopin Radium Institute General Director Alexander Rimski-Korsakov in St. Petersburg, Russia.

Transmutation Research Program Staff, Faculty Researchers and Students



TRP Finance Director
Leisa Rodriguez



Project Assistance
Kathy Lauckner



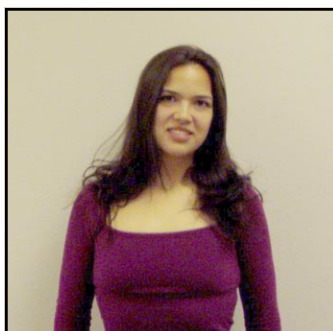
Laboratory Manager
Jeanette Daniels



Finance Assistance
Hallie Lyons



Webmaster
John Knoten



Post Doctoral Researcher
Cynthia Gong



Detector Development
Frank Avignone



David Edwards



Mosese Ohia



Joe Lloren



Erica Summers

Administrative Staff not pictured:

Ruby Bynum
Joe Zimmerman
Michelle Bossler
Kris Davidson
Aishia Henderson
Ran Gao
Karen Bukowski
Kristen Stetzenbach

Task 1:

Yitung Chen
Associate Professor
Associate Director, NCACM
Mechanical Engineering Department

Darrell W. Pepper
Professor, ME Department
Director, NCACM

Randy Clarksean
Adjunct Professor
Mechanical Engineering Department

Students:

Taide Tan
Xiaolong Wu
Yulien Chen
Paul Lawson

Not pictured



Task 2:

Robert A. Shill, Jr. Associate Professor
Associate Professor, Electrical and Computer
Engineering Department



Mohamed B. Trabia
Chair, Mechanical Engineering
Department



William Culbreth
Associate Dean for Research
College of Engineering

Students:

Anoop George
Satishkumar Subramanian
Qin Xue
Myong Holl
Greg Loll



Task 3:

John Farley, Professor
Department of Physics

Dale Perry, Lawrence Berkeley
National Lab, Adjunct Professor

Students:
Dan Koury
Brian Hosterman
Umar Younas
Lindsay Wylie
Denise Parsons

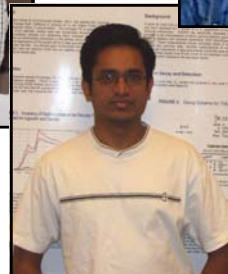
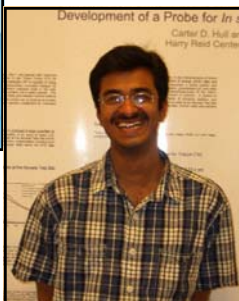
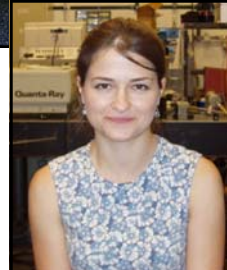
Allen Johnson, Assistant Professor
Department of Chemistry

Students:
Thao Trung Ho
Julie Manzerova
Stacy Sidle
Chris Harland



Task 4 : Ajit Roy, Associate Professor Mechanical Engineering Department

Students: Phandi Gudipati, Mohammad Hossain,
Sudheer Sama, Ramprashad Prabhakaran,
Venkataramakrishnan Selvaraj
Nikata Agarwal and Aaron Tippetts Not pictured





Task 5:

Samir Moujaes
Associate Professor, Mechanical Engineering Dept.

Yitung Chen
Associate Professor
Associate Director, NCACM
Mechanical Engineering Department

Students:

Kanthi Dasika

Chao Wu

Guanjun Li

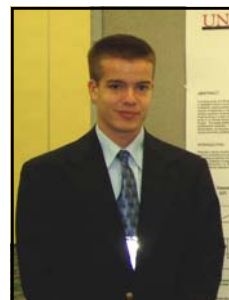
Narain Armbya

Not pictured

Task 6 : Denis Beller, Research Professor Mechanical Engineering Department

Students:

Shruti Patil, Timothy Beller, Dean Curtis, and
Brice Howard



Task 7:

Phillip Patton, Associate Professor

Mark Rudin'
Associate Professor Health Physics

Students:

Deanna Tuttle

Tserenpagma Chaoui

Ashley Gann

Sung Yop Kim

Jeffrey Wyler

Not pictured



Task 8:

Yitung Chen, Darrell Pepper, and Sean Hsieh, faculty, Mechanical Engineering Department

Students: Jianhong Li, Haritha Royyuru and Lijian Sun

Sushma Gujjula and Sridhar Munaga

Not pictured



Task 9:

Georg Mauer, Professor
Mechanical Engineering Department
Caroline Wiejak, visiting scholar.

Students:

Jae-Kyu Lee, Jamil Renno, and Richard Silva



Task 10:

Ajit Roy and Brendan O'Toole, Associate Professors, Mechanical Engineering Department

Students:

Mark Jones, Srinivas Kukatla, Martin Lewis, Venkata Potluri, Bhagath Yarlagadda and John Motaka

Prad Koppula and Raymond Kozak

Not pictured



Tasks 11 and 12:

William Culbreth, Associate Dean for Research
College of Engineering

Denis Beller, Research Professor
Mechanical Engineering Department

Students:

Elizabeth Bakker, Suresh Sadineni
Trevor Wilcox, Daniel Lowe, Robert O'Brien,
Robin Jenkins and Ashraf Kaboud

Not pictured

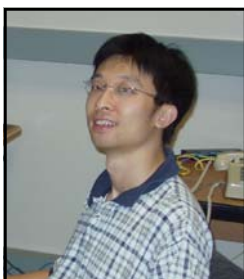


Task 13:

Yingtao Jiang, Electrical and Computer Engineering Department
Bingmei Fu and Jian Ma, Mechanical Engineering Department

Students: Xiaolong Wu
Yi Lu and Shahidur Rahaman

Not pictured



Task 14:

Ajit Roy, Associate Professor, Mechanical Engineering Dept.

Students: Satish Dronavalli, Vikram Marthandam

Anand Venkatesh, Subhra Bandyopadhyay, and Silpa Budugur

Srinivas Chanda

Not pictured



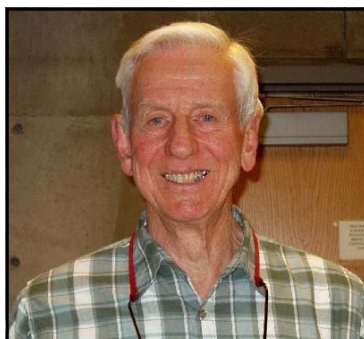
Task 15:

Spencer Steinberg, Professor, Chemistry Department

Gary Cerefice, Assistant Research Professor

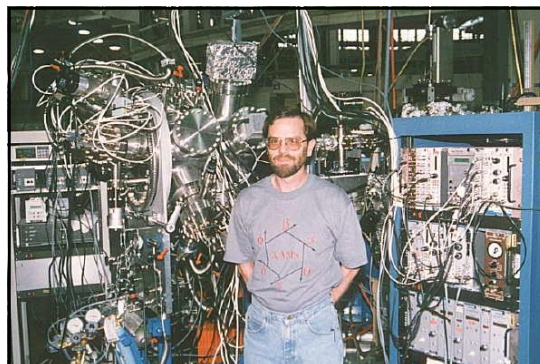
David Emerson, Emeritus Professor

Students: Ginger Kimble and Gregg Schmett



Task 16:

Dennis Lindle, Professor, Chemistry
Oliver Hemmers, Assistant Research Professor, Chemistry
Dale Perry, Adjunct Professor, Physics
Students:
Chirantha Rodrigo and Chinthaka Silva

**Task 17:**

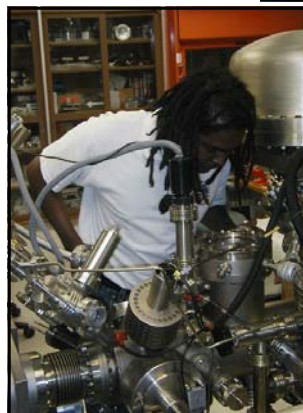
Clemens Heske, Associate Professor, Chemistry

Students:

Goverdhan Gajjala, Timo Hofmann, Kyle George
and Jared White

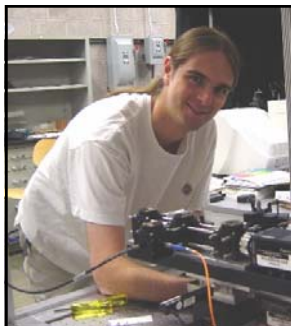
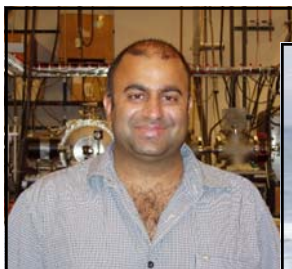
Varun Marepally

Not pictured



Task 18:

John Farley and Dale Perry, faculty, Physics Dept.
Allen Johnson, Assistant Professor, Chemistry Dept.
Students: Umar Younas, Thao Trung Ho, Brian Hosterman
Dan Koury

**Task 19:**

Ken Czerwinski, Associate Professor, Chemistry

Students:

Emil Fridman and Sergei Kolesnikov, Ben Gurion University
Earl Wolfman

**Task 20:**

Ajit Roy, Associate Professor, Mechanical Engineering

Students:

Harish Krishnamurthy, Pankaj Kumar, and
Debajyoti Maitra



Task 21:

Yitung Chen, Associate Professor
Huajun Chen, Postdoc, Mechanical Engineering
Jichun Li, Assistant Professor, Mathematics

Students: Taide Tan and Xianfang Tan



Task 22

Georg Mauer, Professor
Mechanical Engineering Department
Student: Jamil Renno



Task 23

Biswajit Das,, Associate Professor, Electrical and Computer Engineering
Students: Pavan Singaraju and Jonathon Ross

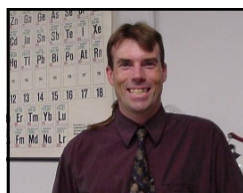
Michael Sadowitz

Not pictured

Task 24:

Yitung Chen, Associate Professor
Sean Hsieh, Research Assistant Professor
Mechanical Engineering Department

Students: Matthew Hodges and Ling Kwan



Task 25:

David Hatchett, Ken Czerwinski and Byron Bennett, faculty, Chemistry Department

Students: Sandra Elkouz, Sujanie Gamage, and Moustapha Eid Moustapha

Not pictured

Task 26:

Ken Czerwinski, faculty, Chemistry Dept.
Students: Amber Wright, (fourth from left) will start the Ph.D. program in Radio-chemistry fall 2005. She is shown with the other AFCI fellows and program administrators.

Inna Bashta

Not pictured



Task 27:

Evgeny Stankovskiy, (far left rear row), Denis Beller (fifth from right in rear row) and Tim Beller, (far right front row) with other attendees at the Third Annual Idaho ADSS Workshop at ISU, Pocatello, Idaho, June 1-2, 2005.

Acronyms

ADS	Accelerator-driven transmutation systems	FCC	transmutation of high level nuclear waste in an accelerator driven system
ADSS	Accelerator-driven subcritical systems	FGR	Fullerene containing carbon
ADTTA	Accelerator-Driven Transmutation Technologies and Applications	FLEX	Federal Guidance Report
AECL	Atomic Energy Canada, Ltd.	FZK	Fluoride extraction process
AES	Auger electron spectroscopy	GTM	Forschungszentrum Karlsruhe, Germany
AFCI	Advanced Fuel Cycle Initiative	GUI	Generic TRUEX Model
AHA	Acetohydroxamic acid	HE	Graphical user interface
AI	Artificial intelligence	HEPA	Hydrogen embrittlement
ALI	Annual limit on intake	HRC	High efficiency particulate air
ALS	Advanced Light Source facility in Berkeley, CA	HTGR	Harry Reid Center for Environmental Studies, UNLV
AMAD	Activity mean aerodynamic diameter	HTMEF	High Temperature Gas-Cooled Reactor
AMUSE	Argonne Model for Universal Solvent Extraction	IAC	High Temperature Materials Experiments Facility, UNLV
ANL	Argonne National Laboratory	ICAPP	Idaho Accelerator Center, Idaho State University
ANS	American Nuclear Society	ICHMT	International Congress on Advanced Nuclear Power Plants
ASM	American Society of Metals	ICONE	International Center for Heat and Mass Transfer
ASME	American Society of Mechanical Engineers	ICOPS	International Conference on Nuclear Engineering
ASTM	American Society for Testing and Materials	ICP-AES	International Conference on Plasma Science
BET	Nuclear data files for beta emitters	ICP-MS	Inductively coupled plasma—atomic emission spectrometer
BOXER	Two-dimensional neutron transport code	ICRACM	Inductively coupled plasma mass spectrometer
CAD	Computer aided design	ICRACM	International Conference on Advanced Composite Material
CAINE	Computer Applications in Industry and Engineering	ICRP	International Commission on Radiological Protection
CEA	French Atomic Energy Commission	IYNC	International Youth Nuclear Congress
CFD	Computational fluid dynamics	IEEE	Institute of Electrical and Electronics Engineers, Inc.
CL	Constant load	IMECE	International Mechanical Engineering Congress & Exposition
CPP	Cyclic potentiodynamic polarization	INL	Idaho National Laboratory
CR	Cold-reduction	ISM	Induction skull melter
CTD	Chemical Technology Division	ISU	Idaho State University
CW	Cold-worked	JEF	Joint European file
DAC	Derived air concentration	JINS	Joint Institute for Neutron Sciences
DBTT	Ductile-to-brittle transition temperature	KRI	Khlopin Radium Institute, St. Petersburg, Russia
DC	Dose coefficient	KRI-KRISI	Khlopin Radium Institute Research Industrial Enterprise, St. Petersburg, Russia
DCAL	Dose and risk calculation software	KWU	Kraftwerk Union
DELTA	Development of Lead-Bismuth Target Applications (test loop at LANL)	LANL	Los Alamos National Laboratory
DHS	U.S. Department of Homeland Security	LANSCE	Los Alamos Neutron Science Center
DOE	U.S. Department of Energy	LBE	Lead bismuth eutectic
DSC	Differential scanning calorimetry	LEED	Low-energy electron diffraction
DTA	Differential thermal analysis	LLW	Low-level waste
ECATS	Experimental Activities on the Coupling of an Accelerator, a spallation Target and a Sub-critical blanket project	LMCE	Liquid Metal Corrosion Experiment
ECS	Electrochemical Society	LWR	Light water reactor
EDAX	Energy dispersive x-ray spectroscopy	MATLAB	A software system integrating mathematical computing and visualization
EDISTR	Nuclear database generator for internal radiation dosimetry calculation	MCNP	Monte Carlo n-particles code
EDS	Energy dispersive spectrometry	MCNPX	Monte Carlo n-particles code, extremely high-energy version
EELS	Electron energy loss spectrometry	MELOX	Mixed oxide fuel fabrication plant, Marcoule, France
EFTEM	Energy-filtered electron microscopy		
%El	Percent elongation		
EMIL	Electron Microanalysis and Imaging Laboratory		
ENEA	Italian Agency for New Technologies, Energy, and the Environment		
ENSDF	Evaluated nuclear structure data file		
EPMA	Electron microprobe analyzer		
EUROTRANS	European research program for the		

MOX	Mixed oxide	SAMPE	Society for the Advancement of Material and Process Engineering
MPI	Message passing interface	SCALE	Standardized Computer Analyses for Licensing Evaluation code
MS VB	Microsoft Visual Basic	SCC	Stress corrosion cracking
MTS	Materials Testing System	SEE	Secondary electron emission
MUSE	<i>Multiplication avec Source Externe</i> project, Cadarache, France	SEM	Scanning electron microscope
NACE	National Association of Corrosion Engineers	SFTF	Spent Fuel Treatment Facility
NCACM	Nevada Center for Advanced Computational Methods, UNLV	SNS	Spallation Neutron Source
ND	Neutron diffraction	SS	Stainless steel
NE	Nuclear Energy, Science and Technology	S-SPA	Structure and Solid Phase Analysis
NICEST	Neutrons in Solid-State Chemistry and the Earth Sciences Today and Tomorrow	SSR	Slow-strain-rate
NMDS	Neutron multiplicity detector system	STAR-CD	A commercial computational fluid dynamics software package
NOM	Natural organic matter	TAMU	Texas A&M University
NTISV	Non-traditional in situ vitrification	TBP	Tributylphosphate
NTS	Nevada Test Site	TC-1	Target Complex 1
NUBASE	A nuclear properties database	TEM	Transmission electron microscope
NURETH	Nuclear Reactor Thermal Hydraulics conference	TGA	Thermogravimetric analysis
OCS	Oxygen Control System	TRADE	TRIGA Accelerator Driven Experiment
OECD/NEA	Organisation for Economic Co-operation and Development/Nuclear Energy Agency	TRISO	A silicon carbide and pyrocarbon composite coating
ORNL	Oak Ridge National Laboratory	TRP	UNLV Transmutation Research Program
PAS	Positron annihilation spectroscopy	TRPSEMPro	TRP System Engineering Model Program
PEELS	Parallel energy loss spectroscopy	TRU	Transuranic actinides
PUREX	Plutonium extraction process	TRUEX	TRU extraction
PVM	Parallel virtual machine	TTF	Time-to-failure
PWR	Pressurized water reactor	UHV	Ultra High Vacuum
PWTT	Post-weld-thermal-treatments	UNLV	University of Nevada, Las Vegas
Q&T	Quenched and tempered	UPS	UV photoelectron spectroscopy
%RA	Percent reduction in area	UREX	Uranium extraction process
RACE	Reactor-accelerator coupled experiment	UT	University of Texas
RBS	Rutherford backscattering spectroscopy	UTS	Ultimate tensile strength
RC	Ring-core	UV	Ultra-violet
RGA	Residual gas analyzer	WIPP	Waste Isolation Pilot Plant, Carlsbad, NM
RSICC	Radiation Safety Information Computational Center	XAES	X-ray auger electron spectroscopy
RSL	Remote Sensing Laboratory	XAFS	X-ray absorption fine-structure spectroscopy
		XML	Extensible markup language
		XPS	X-ray photoelectron spectroscopy
		XRD	X-ray diffraction
		YS	Yield strength
		YSZ	Yttria-stabilized zirconia

References

UNLV Transmutation Research Program references, current activities and other miscellaneous information can be found on the TRP website at <http://aaa.nevada.edu>.

Credits

The University of Nevada, Las Vegas Transmutation Research Program is administered by the Harry Reid Center for Environmental Studies under the auspices of the U.S. Department of Energy (Grant No. DE-FG04-2001AL67358).

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