

2006 SUMMARY OF ENGINEERING RESEARCH

A Report of Activities during 2005

This report is part of the larger *2006 Summary of Engineering Research*, available on the Web at www.engr.uiuc.edu/research and on CD-ROM. The *Summary of Engineering Research* represents the extensive engineering research program conducted in 2005 at the University of Illinois at Urbana-Champaign. Detailed statistics about research in the College of Engineering are included in the *Directory of Engineering and Engineering Technology Programs and Research*, published by the American Society for Engineering Education, Washington, D.C.

How to use the *Summary of Engineering Research*: Research projects are listed by title, followed by the names of the investigators and the sponsoring agencies. Projects are sorted by major topic areas. Project descriptions are brief. Additional information on each project may be obtained from the investigator in charge (denoted by an asterisk). Mailing addresses are provided on the introductory page.

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Abbreviation key for College of Engineering departments and major labs:

- Advanced Transportation Research and Engineering Laboratory (ATREL)
- Aerospace Engineering (Aerosp. Engr.)
- Agricultural and Biological Engineering (Ag. & Biol. Engr.)
- Bioengineering (Bioenr.)
- Chemical and Biomolecular Engineering (Chem. & Biomol. Engr.)
- Civil and Environmental Engineering (Civil & Environ. Engr.)
- Computer Science (Comput. Sci.)
- Coordinated Science Laboratory (CSL)
- Electrical and Computer Engineering (Elect. & Comput. Engr.)
- Frederick Seitz Materials Research Laboratory (FS-MRL)
- General Engineering (Gen. Engr.) or Industrial & Enterprise Systems Engineering (Indus. & Enter. Syst. Engr.)*
- Materials Science and Engineering (Mat. Sci. & Engr.)
- Mechanical and Industrial Engineering (Mech. & Indus. Engr.) or Mechanical Science and Engineering (Mech. Sci. & Engr.)*
- Micro and Nanotechnology Laboratory (MNTL)
- Nuclear, Plasma, and Radiological Engineering (Nucl., Plasma, & Radiol. Engr.)
- Physics
- Theoretical and Applied Mechanics (Theoret. & Appl. Mech.)*

*In August 2006, the Industrial Engineering program was merged with the General Engineering Department, which became the Industrial and Enterprise Systems Engineering Department. The Theoretical and Applied Mechanics Department merged with the Mechanical and Industrial Engineering Department, which became the Mechanical Science and Engineering Department. Please check department links at www.engr.uiuc.edu for current faculty lists.



Nuclear, Plasma, and Radiological Engineering

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Research in the Department of Nuclear, Plasma, and Radiological Engineering is broadly based on issues surrounding the production, transport, and interactions of radiation with matter and the application of all nuclear processes. This includes the traditional areas of nuclear fission for production of electric power as well as nuclear fusion as a near-term scientific tool and as a future energy source.

In addition to these more traditional areas in nuclear engineering, the research efforts in the department now embrace a wide spectrum of plasma science, radiological science, materials science, and other related applications. Also included are topics involving national and global energy and security issues, particularly concerning the development and implementation of nuclear energy sources. These areas reflect the creative interests and breadth of experience of faculty members of the department. These diverse research areas are presented in 13 topical groups.

Primary research directions within the department support the continued role of nuclear power in meeting society's electric power and energy resource needs through currently installed light water fission reactors and through development of advanced reactors, accelerator-based processes, and fusion systems for future applications. Other directions being pursued are broad applications of plasma to materials processing measurement sensing and other processes; development and utilization of radiation sources, including radiological and medical applications; advanced computational and analytical methods; thermal hydraulics and reactor safety; and nuclear materials.

Important contributions have been made recently by several research groups working in the following areas: inertial electrostatic confinement for fusion applications and for neutron, x-ray, and gamma radiation sources;

energy cell performance for heat release and material transmutations; advanced computational techniques applied to stochastic radiation transport, reactor physics, and safety, including Lie groups and group invariant difference schemes; perceptual displays and temporal pattern recognition applied to reactor control and operation; nuclear nonproliferation and safeguards; fusion blanket and diverter materials behavior and performance; plasma processing of electronic materials, plasma-induced sputtering, and plasma measurements; nuclear radiation effects on materials and neutron scattering measurements; materials behavior under high-temperature corrosion and radiation bombardment environments, including nondestructive examination; magnetic resonance imaging for cancer cell treatment; and thermal hydraulics, including multiphase flows, boiling in porous media, molten jet breakup, and turbulent structure modeling; and large-scale computer modeling of fission reactor systems, including reactor and control systems visualization.

Faculty and Their Interests

Roy A. Axford

Application of the Lie Theory of Local Transformation Groups to the solution of linear and nonlinear systems of differential equations that arise in engineering science, theoretical physics, applied mathematics, computational physics of nuclear energy systems

Brent J. Heuser

Hydrogen/metal systems, defects in materials, thin-film structures, numerical simulations of spallation source systems, neutron scattering techniques

Barclay G. Jones

Thermal-hydraulics, reactor safety, multiphase flow, boiling heat transfer, turbulence measurement and modeling, flow-induced vibrations and hydroacoustics, human-machine interfaces for reactor control and simulation, food irradiation-safety

George H. Miley

Fusion systems, plasma engineering, reactor kinetics and control, nuclear pumped lasers, direct energy conversion, hydrogen energy production and fuel cells, low-energy nuclear reactions in solids

Magdi Ragheb

Computational methods, reactor theory, Monte Carlo methods, radiation protection and shielding, probabilistic risk assessment, applied artificial intelligence, supercomputing

David N. Ruzic

Experimental fusion research, modeling of edge plasma atomic physics, atomic properties of potential first-wall materials, plasma-material interaction, plasma processing of semiconductors, extreme ultraviolet (EUV) sources for lithography, physical and chemical vapor deposition

Clifford E. Singer

Energy economics, energy and security, advanced propulsion systems, nuclear proliferation, South and Northeast Asia nuclear programs

James F. Stubbins

Development, analysis, and application of materials, primarily for energy-related applications; nuclear systems design and analysis; nuclear materials, nuclear fuels, irradiation damage and effects, mechanical properties, high temperature corrosion, electron microscopy

Rizwan Uddin

Nuclear reactor theory, homogenization techniques, computational methods, reactor thermal hydraulics, virtual nuclear systems, nonlinear dynamical systems, computational biology

Applied Plasma Physics

Evidence of Hyperstoichiometric Hydride Formation and Superconductivity at Deep Dislocation Cores in Hydrogen Cycled Pd and Pd/PdO Samples

A. G. Lipson, G. H. Miley*

University of Illinois; New York Community Trust

The magnetic characterization of Pd single crystals deformed by cycling in a hydrogen atmosphere has been performed. Based on evidence obtained from thermal desorption analysis, it is shown that the condensed hydrogen phase formed inside deep dislocation cores in PdH_x ($x = \text{H/Pd} \sim 4.5 \times 10^{-4}$) is tightly bound with a Pd

matrix. The activation energy of hydrogen desorption from these cores was found to be as high as $e = 1.6 \text{ eV/H-atom}$, suggesting the occurrence of a strong band overlapping between Pd and H atoms. SQUID measurements carried out in a weak magnetic field ($H < 5.0 \text{ Oe}$) showed an anomalous diamagnetic contribution into DC and AC magnetic susceptibilities of the PdH_x sample at $T < 30 \text{ K}$ resulting in the presence of the hydrogen phase. It is suggested that anomalous diamagnetic response in PdH_x is caused by presence of a hydrogen dominant hyperstoichiometric phase PdH_x ($y \sim 1.35$), tightly bound with a Pd matrix at deep dislocation cores (nanotubes). Transport and magnetic properties have been studied for the novel Pd-Pd oxide material deformed by electrochemical cycling across the hydride miscibility gap. The resulting Pd/PdO:H_x heterostructure contains hydrogen-rich nanoclusters PdH_x ($y \sim 1.8$) trapped along the dislocation cores at the boundary between Pd metal and nonmagnetic PdO oxide. We found significant anomalies of both resistance and magnetic susceptibility in a weak magnetic field suggesting simultaneous appearance of excess conductivity and diamagnetic contribution below 70 K (weak high temperature superconductivity), which is caused by the condensed hydrogen precipitated at deep dislocation cores in the Pd/PdO:H_x sample.

X-ray Laser

G. H. Miley,* A. Khan, I. Percel

U.S. Air Force, FA 9451-04-C-0196

Soft x-ray laser emission has been observed from metal targets such as Ti and Pd, which serves as the cathode in a high-current deuterium glow discharge. This emission is under study in order to better understand the emission mechanism and to explore the possibility of developing a solid-state x-ray laser in the 1 keV energy range. This unique laser provides a shorter wavelength and more compactness than previously reported for tabletop x-ray lasers. The x-ray generation is related to anomalous transfer of energy through recoil events when a highly loaded (D/metal atom ratio) metal hydride is bombarded with a high current ion beam. Then energy associated with the deuteron desorption/flow from the overheated cathode surface creates nonequilibrium lattice phonons, which excite a metastable super-cell state in the loaded metal.

* Denotes principal investigator.

Debris Mitigation for EUV Semiconductor Processing Sources

D. N. Ruzic,* S. Srivastava,* E. Antonsen,*
M. Jaworski, K. Thompson
Intel Corporation, Intel SRA 03-159

As semiconductor photolithography techniques become more demanding in 2009–2015, next-generation plasma-based light sources are required to attain 1-10 nanometer-scale feature sizes. A leading candidate for generating this extreme ultraviolet light is a dense plasma focus (DPF). The DPF, originally used for fusion research in the 1960s–1980s, is ideal for creating a point source of light required for the complex optics and lithography masking process. For a DPF light source to become economically viable, it must possess repeatability, long-lifetime, and high availability. The IDEAL (Illinois Debris-mitigation for EUV Sources Applications Laboratory) testbed facility has been constructed to research schemes for reducing debris, limiting erosion, and improving electrode lifetime for a DPF 13.5 nm light source with secondary RF plasmas, foil traps, and biased collectors.

Development of an Internal Helicon Antenna

D. N. Ruzic,* B. Masters
University of Illinois

Helicon plasmas are constructed in nonconducting chambers because the coil “must” be on the outside of the device. The helicon waves must be able to pass through from the antenna to the plasma and the antenna cannot be shorted. Using glass or quartz chambers are problematic though due to vacuum problems and temperature limits. Our idea is to try to place the coil inside the chamber and therefore inside the plasma. The thought is that the coil could be insulated itself and even produce plasma on the exterior of the coil. A variety of antenna shapes are being studied and probes are being used to determine if helicon waves are still present.

Gibbsean Alloy Development for EUV Mirrors

D. N. Ruzic,* H. Qiu, A. Rockett*
Intel Corporation, Intel SRA 03-159

One possible way to extend the lifetime of the optics used in extreme ultraviolet (EUV) manufacturing is to produce an alloy that will self-heal. Under ion bombardment, the top surface of the mirror is removed, or “sputtered” away. This could drive a surface-concentration gradient, alloying a minority species to segregate to the surface. We have set up an experiment to produce such alloys. Our first attempts have been using gold to segregate to the surface of molybdenum. For the technique to work properly, extreme

care must be paid to impurities in the film. Several impurity reduction techniques are being researched.

Incorporation of Fractal Geometry into Surface Reflection and Sputtering Monte Carlo Codes

D. N. Ruzic,* M. Coventry, D. Alman, H. Qiu
National Science Foundation, DMR-9201689

Seacoasts, clouds, mountains, and the microstructure of surfaces can all be described by fractal geometry, a geometry not limited to integer dimensions. Present surface analysis computer models such as TRIM and the “embedded atom method” treat surfaces as flat. They calculate the reflection coefficient and sputtering coefficients as a function of energy, angle of incidence, and material composition. This study introduces realistic surface roughness and more complete interaction physics into those codes by incorporating the fractal geometry concept.

Lifetime of Optical Components in EUV Systems

D. N. Ruzic,* E. Antonsen,* S. Srivastava,*
K. Thompson
Xtreme Technologies

A commercial high-power extreme ultraviolet (EUV) source utilizing a fast Z-pinch Xe plasma is used at Illinois to simultaneously expose sample mirrors and test techniques of debris mitigation. This source is a prototype of the type that will be used by semiconductor manufacturers to make the 32-nm node of semiconductor chips. These will be in computers available in the year 2009 and be roughly 10 times faster and smaller than the computers in use today. The experiment will determine which mirrors live up to the harsh environment and help find ways to extend their lifetime.

Measurement and Simulation Damage to Reflective Surfaces

D. N. Ruzic,* S. Srivastava,* H. Qiu, H. Shin
Intel Corporation, Intel SRA 03-159

Extreme ultraviolet (EUV) radiation is accompanied by fast ions and neutral atoms that can damage mirror surfaces. The fuel atoms and electrode material for the source can also be present and coat these same mirrors. An investigation has been launched into the surface morphology, composition, and depth characteristics to learn more about the damage mechanisms and how effective certain mitigation schemes can be. The U.S. Department of Energy supported Center for Microanalysis is also involved in this work.

* Denotes principal investigator.

Measurements of Ion-Induced Electron Emission, Reflection, and Sputtering

D. N. Ruzic,* M. Coventry

U.S. Department of Energy, DE-FG02-99ER54515

When ions strike materials, electrons may be emitted, the ion reflected, or the material removed (sputtered). Magnetron sputtering is useful in all microelectronics and the production of videocassette tapes. In a magnetron, plasma ions fall through the plasma sheath and impact the target. The emitted electrons are accelerated away from the target and sustain the plasma discharge; the sputtered material deposits on the microelectronic device being fabricated. To understand this system in detail, the emission coefficients for low-ion energy must be known. These measurements are complicated by the presence of real-life adsorbates and surface defects. Measurements of these phenomena are under way in a UHV ion-surface interaction facility. Modeling efforts are also under way.

Modeling of Spectra Intensities and Time Evolution from Pinch Plasmas

D. N. Ruzic,* S. Srivastava,* J. Spencer

Starfire Industries

Extreme ultraviolet (EUV) light used in advanced semiconductor manufacturing, biological “water-window” microscopes, and other applications is produced in plasma pinches. These are initiated by either a laser firing at a solid target, or by a plasma. In either case, the dynamics of the evolving plasma need to be modeled so that the light emission can be simulated. We are working with advanced spectral codes to predict the pinch parameters most favorable to the highest production of the required EUV light. In addition, we can predict the ion energy spectra emitted.

Multiprocessing Chamber for Etching and Deposition in Semiconductor Manufacture

D. N. Ruzic,* J. Norman, M. Neumann, N. Li

LSI Inc.

For computer chips to continue to become faster, better, and cheaper each year, machines must be made to produce them. To date, this has meant that each step of the process has become more complicated, requiring more and more specialized apparatus. Soon the cost of making improvements in this way will outstrip the advances made, and computer chips may get smaller, but they will not be cheaper. A focus of this research is on creating one processing chamber that can accomplish more than one of the processing steps. Through advanced diagnostics and control of the helical-wave generated plasma, a machine

such as the one used in this research may keep down the costs of future computer chips.

Particle Removal from Masks and Wafers

D. N. Ruzic,* M. Neumann, H. Shun, W. Lytle

Intel Corporation; ASML Corporation

The particle contamination on extreme ultraviolet (EUV) surfaces during mask blank deposition, mask fabrication, patterned mask handling can create significant distortions and loss of reflectivity and must be avoided. Particles on the order of 10nm are problematic during MLM mirror fabrication, since the introduced defects disrupt the local Bragg planes. The most serious problem is the accumulation of particles on surfaces of patterned blanks during EUV light exposure, since >25nm particles will be printed without an out-of-focus pellicle. Particle contaminants are also a problem with direct imprint processes since defects are printed every time. Several plasma-based techniques are under investigation aiming to reduce particle contamination through the use of controlled electrostatic repulsion and expulsion of particles from surfaces. The preliminary experiment simulates the particle contamination of mirror samples by introducing external insulating nanoparticles of <200 nm size (PSL). Local charging of the particles is governed by the application of a plasma, electron beam, and voltage bias on the substrate. Coulomb explosions and Malter effects that cause surface damage are minimized or eliminated by precise control of the local environment. Data from several plasma schemes to remove particles will be presented, including the first experiment demonstrating the removal of >85% of particles. Particles are imaged with a high-resolution SEM and numerically counted using contrast information from the image histogram. The capabilities for extending this process to higher levels suitable for manufacturing are being researched.

Selective Etching of EUV Mirror Components

D. N. Ruzic,* S. Srivastava,* H. Shin

Intel Corp., Intel SRA 03-159

Collecting the light from extreme ultra-violet (EUV) sources is an essential step in making EUV lithography a reality for semiconductor manufacturing in the 2009- 2015 period. The optics needed for this task consist of multilayer mirrors that use Bragg reflection to get almost 70% reflectivity at the 13.5 nm wavelength. Unfortunately the leading source material that emits the light in this wavelength is tin. Tin-containing gasses are fed into a plasma-based source to produce the EUV light. The tin atoms have to go someplace. Despite mitigation, some of them will end up on the multilayer mirrors. Even very thin

* Denotes principal investigator.

layers less than 10 nm thick will ruin the reflectivity. Therefore, some sort of *in situ* cleaning is needed. This research focuses on a new technique to do the *in-situ* etching of tin simultaneously with the exposure without etching the multilayer mirrors themselves.

Surface Cleaning of EUV Optics by Plasma Exposure

D. N. Ruzic,* M. Neumann

Cymer Corporation

A critical step in the manufacture of semiconductor chips is lithography—the patterning of the circuit design onto the chip. As features have grown smaller, the wavelength of the light used for the lithography must also shrink. Extreme ultraviolet (EUV—13.5 nm light) will be used for the 2009 generation of chips. These wavelengths can only be made using a plasma, which creates a considerable number of energetic particles and low-energy contaminants. The first optical element that collects the photons will be subject to these fluxes and may lose its reflectivity. We have built an experiment, SCOPE (surface cleaning of optics by plasma exposure), to simulate the ion damage, deposition, and potential plasma-based cleaning techniques that could be used to ensure sufficient lifetime of these collectors.

The Measurement and Control of High-Aspect-Ratio Etching for Semiconductor Applications

D. N. Ruzic,* E. Ritz

Micron Corporation

The most advanced memory chips have very high aspect ratio (20:1 or greater) features. To produce those features, they must be etched with an unusually high degree of anisotropy. Problems can occur in the process due to differential charging on the sides vs. the bottom of the trench or via. Experiments are under way to measure such charging and then to devise a pulsed plasma technique to eliminate its detrimental effect.

Arms Control, Disarmament, and International Security

South Asia, an Area of Continuing National Security Concern

C. E. Singer*

U.S. Department of Defense National Security Education Program, DASW01-00-1-0007

Researchers with the Program in Arms Control, Disarmament, and International Security (ACDIS) at the University of Illinois are working in cooperation with the Department of Engineering and Public Policy at Carnegie Mellon University and the Center for International Trade

and Security at the University of Georgia at Athens. This innovative program in South Asian security studies combines the study of language and culture with an examination of major security issues, including environmental concerns, uses of nuclear energy, and international trade policy.

Strengthening Scientific and Technical Advice on International Peace and Security Policy

C. E. Singer,* E. D. Kellogg (International Programs and Studies)

John J. and Catherine T. MacArthur Foundation, 02-747538-GSS

This program focuses on three areas: chemical and biological agents, cyberwarfare and cybersecurity, and technologies relevant to nuclear and other weapons of mass destruction or disruption and their means of delivery. The objectives of the program are to recruit and support new faculty in science and technology with research and teaching interests in international peace and security; foster interdisciplinary graduate study related to technology and security policy through course development, mentoring, and fellowships; provide research associate and visiting scholar opportunities; and bring university researchers together with the policy community in an annual conference and other forums to address international peace and security.

Chemical Reaction

Chemical Reactions in Nano-Confined Volumes

G. H. Miley,* D. Noid*

Oak Ridge National Laboratory

Current research involves theoretical study of chemical reactions in nano-confined volumes, especially in issues involving the forces between molecules in metallic nanocavities. Molecular forces involved include the nonbonded interactions between nonpolar molecules due to photon-mediated interactions. Force carriers may be modified or even attenuated since consequently, new interactions are conceivable that would not exist in the gas phase. In addition to theoretical analysis, a possible experiment involving nano bubbles in a liquid metal are under consideration.

Molecular Mossbauer Effect

G. H. Miley,* D. Noid*

Oak Ridge National Laboratory

Recent experiments have reported extraordinary interactions between ultracold neutrons with

* Denotes principal investigator.

biomolecules. The high recoil energies of the hydrogen atoms absorbing a neutron apparently cause large-scale molecular fragmentation. Consequently, the effect of such high energy/frequency interactions are under study with molecular dynamics methods that have been adapted to very short time scales and high energies. Modifications involve changing the interactions terms between bonded atoms for a time scale where chemical forces are not relevant (electron exchange not possible). The resulting dynamics reveal a new type of molecular Mossbauer effect that, coupled with electronic wave function transfer to the nonbonded state, could explain the experimental results.

Computational Mechanics

Hybrid Scheme for Multigroup Neutron Diffusion Equations on Arbitrary Geometry

R. Uddin,* Y. Gu

U.S. Department of Energy; Penn State University, DOE PSU 2406-UI-4423

Next-generation research reactors and GEN-IV power reactor designs may require the solution of multigroup neutron diffusion equations in geometries to which the standard nodal schemes, that have been in use for several years, may not apply. Taking advantage of the successful development of the hybrid scheme for the heat conduction, convection diffusion, and the Navier–Stokes equations, we are now extending the idea to solve multigroup neutron diffusion equations in arbitrary geometries. As in earlier applications, the domain is divided into rectangles and triangular nodes (cells). The conventional nodal integral method (NIM) is being applied to the interfaces between adjacent rectangular nodes (cells), while a finite analytic approach is developed for the interfaces between rectangular and triangular nodes (cells). Different basis functions are being explored for the triangular cells. Preliminary results for source and criticality problems are encouraging. This work is now extended to the transport equation.

Hybrid Scheme for Navier–Stokes Equations in Arbitrary Geometry

R. Uddin,* A. Toreja

U.S. Department of Energy, Center for Stimulation of Advanced Rockets; and University of Illinois

A hybrid nodal-integral/finite-analytical method (NI-FAM) is developed for time-dependent, incompressible flow in two-dimensional arbitrary geometries. In this hybrid approach, the computational domain is divided into parallelepiped and wedge-shaped space-time nodes (cells).

The conventional nodal integral method (NIM) is applied to the interfaces between adjacent parallelepiped nodes (cells), while a finite analytic approach is applied to the interfaces between parallelepiped and wedge-shaped nodes (cells). Method developed in this research has been applied to several fluid flow problems including flow in an enclosed cavity. Results are compared with those obtained using a commercial computational fluid dynamics code.

Parallel Modified Nodal Integral Method for 3-D, Time-Dependent, Navier–Stokes Equations

R. Uddin, S. Singh

U.S. Department of Energy, Penn State University, DOE PSU 2406-UI-4423

A modified nodal integral method (MNIM) for 3-dimensional, incompressible Navier–Stokes (N-S) equations has been recently developed. The MNIM code for the N-S equations has now been extended to run on parallel clusters. Since a template of the nodal integral method is quite different from those that result from finite difference or finite volume schemes, parallelization of a nodal code has unique challenges. One objective of this research is to identify characteristics and features specific to parallelization of nodal schemes and to demonstrate that parallel MNIM has speedup and efficiency comparable to other methods (for example finite volume method). Parallel MNIM is applied to practical natural convection cooling problems in next-generation nuclear reactors.

Simulation of Aerodynamic Characteristics of Trailers

R. Uddin,* S. Singh, D. Pointer (ANL)

Argonne National Laboratory, DOE-ANL 4J-00181-003A

The goal of this project is to develop guidelines for using available commercial CFD codes by heavy vehicle industry. The CFD codes are being used for evaluating drag coefficient as well as surface pressure distribution. The guidelines are developed by comparing numerical results with measured drag coefficients and surface pressure distribution from wind tunnel experiments carried out at the NASA Ames Laboratory using a 1/8th-scale conventional U.S. tractor-trailer geometry. The study is used to evaluate effect of global as well as near-surface mesh size parameters. In addition, selection of turbulence modeling strategies is also considered. The project is in collaboration with U.S. DOE Aerodynamic Drag Reduction Team, Argonne National Lab.

* Denotes principal investigator.

A Nodal Scheme for Turbulent Flows

R. Uddin,* S. Singh

U.S. Department of Energy, Argonne National Laboratory 4J-00181-003A; U.S. Department of Energy Penn State University 2406-UI-4423

Designs of next-generation research reactors as well as next-generation nuclear power plants are expected to take full advantage of recent developments in computational fluid dynamics. Computational tools are being developed to perform thermal hydraulics analysis of future designs. Successful application of the nodal integral method to time-dependent Navier–Stokes equations has led to this exploratory research. Our goal in this research is to extend the nodal scheme developed earlier for the Navier–Stokes equations to turbulent flows. Turbulence is being modeled using k-epsilon and LES models. Corresponding discrete equations for the new variables in the k-epsilon model are very similar to those obtained earlier for u , v , and w velocities.

Health Physics, Radiological, and Medical Applications

Medical Dosimetry Planning and Determination

R. Nelson,* J. Stubbins,* M. Garada

Provena Covenant Medical Center, 99-241

This project is to develop efficient methods for planning patient dosimetry for radiation oncology applications using accelerator beams. The work is carried out in conjunction with a local hospital, and the applications are clinical in nature.

The Control of Porosity and Biological Properties of Medical Plastics through Plasma Processing

D. N. Ruzic,* M. Neumann

INTEL Corporation, INTEL SRA 03-159

Many medical applications care about the interaction of biology on materials used in the body. This could be a catheter, or a heart valve, or even a drug introduction system (time-release capsules, for example). The use of plasma processing to alter the surface of many biocompatible materials is just now being explored. This research may lead to new control of porosity and biofouling while keeping the process temperatures low. The use of an ECR and Helicon-wave plasma processing reactor on many potential substrates demonstrates the ability of this new technology to contribute to the biomedical field.

Targeting Ion-Chelate Complexes to Tumors and Tumor Cells

E. Wiener*(Univ. of Pittsburg); J. F. Stubbins*, M. Forbes

University of Illinois

Ion-chelate complexes have many applications in tumor diagnosis and therapy. Radioactive isotopes of technetium, yttrium, indium, and samarium offer applications in radioscinigraphy and radiotherapy. Gadolinium has applications in magnetic resonance imaging and neutron capture therapy. Researchers have attached ion-chelate complexes to Starburst™ dendrimers. Folic acid was attached to these polymers. They specifically bind to tumor cells that express the high affinity folate receptor. The team is using these polymers to diagnose and treat tumors that express this receptor *in vivo*. Tumors of epithelial origin express this receptor. These include 90% of ovarian tumors, ependymomas, and choroid plexus tumors.

Low-Energy Nuclear Reactions

First Principles Studies of Proton Flow in Metals Highly Loaded with Hydrogen

G. H. Miley,* N. Luo

University of Illinois

The nature of hydrogen transport in metals such as palladium is investigated in this research. Drift experiments strongly suggest that H drifts in Pd in the form of a positive ion with a fractional charge number around $+0.5 \sim 0.7$, which gives support to the so-called proton model in which the hydrogen is assumed to be largely ionized. However, experiments on electronic specific heat show that such a proton model is oversimplified. First principles methods, which means calculations without fitting parameters, were used to study the electronic structures of palladium hydrides (PdH). The charge state of H at different sites and at various H compositions (loadings) was calculated by using the so-called full potential linearized augmented plane wave (FLAPW) technique. The result shows that the positive fractional charge manifested in the drifting experiment is a pure dynamic effect because hydrogen at a general site usually shows large accumulation of negative charge in static state. H drifting appears to involve a partially charged positive ion because the proton attracts some extra negative charge in its hopping path, which partially screens out the unit positive charge carried by the proton. The result qualitatively agrees with the experiments.

* Denotes principal investigator.

Low-Energy Nuclear Reactions in Thin Films

G. H. Miley,* N. Luo, C. Castano, T. Woo

University of Illinois

Experiments and theoretical studies are being carried out to study an electrolysis process (or a high pressure process) to force hydrogen atoms into the lattice structure of thin film (500 to 3500 Å) of metal such as Ni and Pd. In this manner a very high loading, approaching 1 atom H/atom metal, is achieved, which is a necessary condition for low-energy nuclear reactions LENRs to occur. In addition, the experiments are designed to create a high flow of protons through the lattice. The metal films are analyzed.

Calorimetric studies are performed before and after the experiment, to establish the signatures of LENRs to measure the energy output of the thin films. The ultimate goal of this research is to understand the basic physics of LENRs.

Nuclear Fusion

Collision Modeling of Inertial Electrostatic Confinement (IEC) Systems

G. H. Miley,* R. Stubbers

University of Illinois

IEC devices typically run at low gas pressures (1-10 mTorr), which provide a plasma that is mostly collisionless. However, the collisions that do occur, especially charge exchange, significantly alter the ion energy distribution within the IEC. This in turn affects the fusion rate. Computational studies have been undertaken to determine the effects of charge exchange, impact ionization, and other collisions in an IEC device.

Preliminary results indicate that under typical conditions, the average ion energy is reduced to 80% of the applied voltage for small (1 cm radius) grids and 60% for larger (3 cm radius) grids. This computational model is now being used to optimize the IEC design so that collisional losses are reduced, maximizing the neutron yield.

Computational Database for Charge Exchange and Ion Stripping in Heavy Ion Beam (HIB)

G. H. Miley,* H. Momota, L. Wu, H. J. Kim

U.S. Department of Energy

This research focuses on developing a subroutine for the LSP code that is widely used for beam transport simulation in Heavy Ion Beam (HIB) fusion research. This subroutine will provide input data on charge exchange and ion stripping, especially multielectron processes for use in near-term HIB experiments and future drive-scale power units. Data mining and numerical calculation results are

being combined to build an evaluated database with the subroutine for the use of LSP code. Further numerical calculations are needed in Phase II to fill in gaps for unsolved data. Representative stripping and recombination reactions have been selected for use in the prototype code. The research will make LSP more capable for use in HIBF studies, including near-term experiments, and will help in design of the next step to build an HIB demo reactor.

Instability Studies on a Spherical Inertial Electrostatic Confinement

G. H. Miley,* H. J. Kim, H. Momota

Department of Energy

Inertial electrostatic confinement (IEC) offers an alternative fusion plasma confinement scheme. It is very attractive for a power plant due to its mechanical simplicity and high power-to-mass ratio. However, various stability issues must be resolved before reactor feasibility can be established. Such stability studies are the objective of the present study. In order to evaluate the IEC concept, it is essential to develop a reliable and flexible instability analysis method for an equilibrium plasma in a potential well. As a part of this study, methods will be sought to avoid or suppress any destructive instabilities. Methods to be explored will include modification/control of the well profile, control of the electron to ion beam density ratio, control of the angular momentum of the beam, etc. For this purpose, a perturbative particle simulation technique for a kinetic analysis will be applied to simulate completely the dynamic evolution of perturbed Vlasov-Poisson equations and, in addition, to achieve much more accurate simulations of the nonlinear dynamics using less simulation particles compared to the conventional particle-in-cell (PIC) method. This model will be used to study the behavior of two-stream-like instabilities related to the trapped spherically converging ions. Then, stability boundaries in various operating parameter spaces will be presented.

Spherical and Cylindrical Inertial Electrostatic Confinement (IEC) Fusion Research

G. H. Miley,* H. Momota,* R. Stubbers, J. Webber,

L. Wu, H. J. Kim, Y. Yang

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NAS8-02012; NPL Associates, Inc.*

The IEC uses a central cathode grid to ionize a low-pressure gas within either a spherical or cylindrical vacuum chamber. Ions are extracted and accelerated to high energies by the grid and are focused at the center of the chamber, creating a high density fusing plasma core. Experiments have yielded over 108 steady state DD fusion

* Denotes principal investigator.

neutrons per second in both configurations. The objective now is to further improve performance by pulsed high-current operation for greater fusion neutron yield. Other studies include investigation of forced and natural plasma oscillations for plasma core densification and study of electrode grid and insulator design for increased ion confinement and for grid lifetime extension. Also under investigation is UVU light emission using ion-rare gas halide interactions for possible light source applications.

A Dipole Assisted Inertial Electrostatic Confinement (IEC) Neutron Source

G. H. Miley,* H. Momoto, P. J. Shrestha
U.S. Department of Energy

Existing inertial electrostatic confinement fusion devices are not yet efficient due to current limitations attributed to ion confinement time, low reaction rates, and electron loss rates. These limitations may be overcome by combining particular IEC confinement geometries with the advantages of the closed field line system of a magnetic dipole. This project seeks to determine an optimized Dipole-IEC configuration and verify the increased confinement times, reaction rates, and energy efficiency that such geometries are reasoned to provide. A more efficient Dipole-IEC confinement system could provide a fast track for development in the short term as a commercial fast-neutron source suitable for medical isotope production, weapons detection, and industrial applications. A Dipole-IEC will also yield an improved understanding of the plasma physics of both IEC and magnetic dipole confinement.

A Traveling Wave Direct Energy Converter for Advanced Fusion

G. H. Miley,* H. Momota; M. Ishikawa, (Tsukuba Univ.)
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The principle of the traveling wave direct energy converter mechanism is understood as a combination of a traveling wave tube and a linear accelerator. The 3-D numerical simulations are being carried out to optimize device parameters. Self-excitation of an alternative electric power in the transmission circuit was examined with a theoretical analysis as well as by 3-D numerical simulations. Based on parameters from a conceptual reactor study, a conversion efficiency of over 70% is predicted. This concept has been employed in recent studies of inertial electrostatic confinement (IEC) space propulsion. In that case, IEC fusion power is converted to electricity for use in ion thrusters.

Design Considerations for the Edge Region of Next-Step Fusion Devices

D. N. Ruzic*
U.S. Department of Energy, DE-FG02-89ER52159

Russia, Japan, Western Europe, and the United States are jointly designing a tokamak reactor that will achieve and sustain fusion ignition. One region of particular concern is the edge region where the plasma strikes the wall. The helium produced by the fusion events must be exhausted, and the power load must not melt the wall and contaminate the plasma. New ideas which may make this possible include lithium walls and flowing liquid concepts for the divertor. Complete modeling of this edge region, including the detailed macroscopic and microscopic geometry and neutral atom scattering, is of critical importance as well.

ELM- Simulating Plasma Gun

D. N. Ruzic,* T. Gray, B. Masters
U.S. Department of Energy, DE-FG02-99ER54515

Modern tokamaks suffer from “edge-localized modes” otherwise known as ELMS. These are rapid bursts of plasma that leave the edge of the device and strike the walls causing erosion and impurity productions. As machines scale up in size, these ELMS are expected to be the limiting factor in performance. To simulate these phenomena, we have built a plasma gun that can shoot blobs of plasmas similar in many characteristics to ELMS. These blobs will interact with a target in a strong magnetic field and allow us to make detailed measurements of the plasma shielding and other phenomena that may occur, thus leading to solutions for fusion devices.

FLIRE: Flowing Liquid Metal Illinois Retention Experiment

D. N. Ruzic,* T. Gray, B. Masters, M. Jaworski, P. Brenner
U.S. Department of Energy, DE-FG02-99ER54515

Future fusion devices will have very high heat loads that could melt the walls of the fusion device. The use of a flowing liquid not only allows for rapid heat removal, but also lets the wall be replaced continually. Though this concept has much merit, there are several unknowns about the interaction of a plasma with a flowing liquid metal. Will the incident hydrogen and helium be retained? If so, for how long? Retaining some helium is a must: otherwise, a fusion device would eventually choke on its own waste products. Retaining too much hydrogen could be very bad, though, because refueling can be difficult. Here at the University of Illinois, researchers are building FLIRE, a laboratory-scale experiment that will measure these

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retention properties and answer other important questions about the feasibility of this new concept.

Kinematic and Thermodynamic Effects on Liquid Sn Erosion

D. N. Ruzic,* M. Coventry, H. Qiu

U. S. Department of Energy, DC-FG02-99ER54515

Fundamental studies of erosion from materials in the liquid phase are studied in the ion-surface interaction experiment (IIAX). Erosion dependence on temperature and surface chemical state is studied for a variety of liquid metals, including lithium, tin, and tin-lithium. The nonlinear behavior of sputtering from liquid lithium surfaces opens the question of whether the coupling of kinematic and thermodynamic mechanisms can lead to a nonlinear change in sputtering when the system temperature is changed. Molecular dynamics models as well as binary collision models are used in this work.

Measurements of Plasma Interactions with Liquid Metals

D. N. Ruzic,* R. Stubbers, T. Gray, B. Masters, B. Schultz, P. Brenner

U.S. Department of Energy, DE-FG02-99ER54515

One of the critical technological challenges of future fusion devices is the ability for plasma-facing components to withstand high power densities. One alternative addressing this challenge is the use of free surface flowing liquids as plasma-facing components (PFCs). Some examples of these free surface liquids include liquid-metals, such as liquid lithium, and nonconducting fluids, such as flibe (LiF-BeF₂). Hence, the understanding of free surface flowing liquid-plasma interactions and associated boundary plasma physics, boundary particle fluxes, bulk liquid-metal diffusion, and surface properties is indispensable in the development of advanced plasma-facing components for future generation fusion machines. The Flowing Liquid Surface Illinois Retention Experiment (FLIRE) has been built to perform experiments that provide fundamental data on the retention and pumping of He, H, and other species in flowing liquid surfaces. FLIRE is a dual-chamber unit, and these two chambers become effectively isolated once the lithium starts to flow. In the first chamber, an ion beam or a DC plasma injects ions at nearly normal incidence into a flowing stream of liquid lithium: the liquid lithium flows into one vacuum chamber isolating it from a bottom vacuum chamber, where the ions released from the metal can be detected by a residual gas analyzer with a quadrupole mass spectrometer. The release rate of gas in the bottom chamber can be used to calculate retention coefficient (ratio of injection rate to release rate)

and the diffusion coefficient. FLIRE also has the capability of studying long-term trapping of reactive gases (i.e. H) and surface desorption kinetics by the thermal desorption spectroscopy (TDS) technique.

Study of Breakdown of Gases in Antennas for the Injection of Radio Frequency (RF) Energy in High-Temperature Plasmas

D. N. Ruzic,* C. H. Castano, M. Aghazarian

Oak Ridge National Laboratory, U.S. Department of Energy

The study focuses on the breakdown characteristics of different gases utilized in waveguides and radio frequency (RF) antennas as feedthroughs for fusion plasma energy injection. The parameter space includes variations of electrode material, surface preparation, magnetic and electric field strength, electrode geometry, and gas pressure. The objective is to understand better the fundamental arcing mechanisms and the effect of surface gas coverage to increment the power rating of antennas for the injection of energy into fusion plasmas.

Nuclear Materials, Materials Science and Performance, Radiation Effects, and Waste Management

Coherent X-Ray Diffraction Measurements of Strain Associated with Embedded Hydride Particles

B. J. Heuser, H. Ju

National Science Foundation

The direct measurement of local lattice strain associated with a single metal hydride particle embedded in a host matrix with coherent x-ray diffraction (CXD) is proposed. The ability to isolate a single second phase particle and study coherency loss directly by quantifying local strain states would represent a significant advancement in materials characterization. Coherent x-ray diffraction is a relatively new technique that is only practical at 3rd generation synchrotron x-ray sources like the Advanced Photon Source. This technique can, in principle, provide a direct measurement of lattice strain specific to a single particle. We are attempting the first such experiment designed to measure the loss of coherency strain during hydride formation.

* Denotes principal investigator.

Extreme Ultraviolet Light (EUVL) Optical Element Performance

B. J. Heuser*, M. M. C. Allain, H. Ju,
J. P. Allain (Argonne National Lab)
Argonne National Laboratory (ANL)

The performance of UV light optical elements has been investigated with x-ray reflectivity. The optical elements are necessary to collect light in the UV range for next-generation lithography devices. These devices use energetic plasmas as the source of UV light and plasma debris are expected to degraded performance over time. We are using x-ray reflectivity measurements under a wide variety of energetic ion bombardment conditions to characterize the influence of the plasma on performance.

Hydrogen Incorporation into Ni-Ti Neutron Supermirrors

B. J. Heuser*, H. Ju
Innovations in Nuclear Engineering Infrastructure in Education (INIE), U.S. Department of Energy

Neutron supermirrors are optical devices based on total external reflection that allow low energy neutrons to be transported over tens of meters without significant loss. Most solids and liquids with sufficient surface smoothness will total-reflect neutrons below a certain critical angle. The critical angle is increased when metal bilayers are deposited. Such multilayer film architectures are called supermirrors. We are currently characterizing Ni-Ti multilayer depositions grown at the University of Illinois at Urbana-Champaign with x-ray and neutron reflectivity. The performance of these depositions will be compared to similar depositions with hydrogen added to the Ti. The goal is improved performance resulting from an increase in the neutron scattering length density contrast between the Ni and hydrogen-containing Ti.

Hydrogen Phase Behavior in Thin-Film Metals

B. J. Heuser*, A. Celik-Aktas
National Science Foundation, DMR-9982520

Transmission electron microscopy is being used to directly observe hydride formation in thin-film Pd. Of particular interest to us is the incoherent nature of Pd hydride, and one goal is to observe the propagation of the phase boundary directly during *in situ* exposure. A second aspect of the work is to determine the influence of dislocations on the hydride formation process. The hydride formation-decomposition process in Pd is known to have a significant hysteresis. Another goal of this project is to determine what microstructural features may influence the hysteresis.

Hydrogen Phase Behavior in Thin-Film Metals

B. J. Heuser*, M. M. C. Allain
National Science Foundation

The phase behavior of hydrogen is altered in restricted geometry like metal thin films. We are interested in this phenomenon and are using x-ray diffraction to characterize phase separation in the hydrogen-epitaxial niobium system. Niobium grows nearly strain free on a-plane sapphire, making this an ideal system to study the interplay between lattice strain and phase separation. Results of the x-ray diffraction measurements indicate two regimes of lattice strain response, a thin-film regime and a thick-film regime. Films in the former respond as ideal, clamped elastic media, while films in the latter act as pseudo-bulk media where plastic instability is manifested as a bulk-like elastic response that is actually anisotropic in nature. This work has unified experimental results of several groups worldwide over the last 15 years.

Hydrogen-Induced Diamagnetic Contribution to the Paramagnetic Response of Deformed Pd

B. J. Heuser*, L. H. Greene* (Physics)
University of Illinois Research Board

Magnetic susceptibility and electrical resistivity are important properties of materials that influence the performance in a wide variety of applications. We have investigated the magnetic susceptibility and electrical resistance of deformed single crystal Pd with low concentrations of hydrogen down to 4 K. A low-temperature diamagnetic contribution to the paramagnetic response of Pd has been observed. This observation is consistent with a type II superconductor, possibly resulting from a condensed hydrogen-rich phase along dislocation cores in the deformed Pd matrix.

Neutron Transport in Spallation Neutron Source Target-Moderator Assemblies

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J. M. Carpenter (Argonne National Lab.)
National Science Foundation (subcontract from University of Tennessee), OR 11361-01

The development of advanced accelerator-based neutron sources, such as the Spallation Neutron Source (SNS) at Oak Ridge National Laboratory, has ushered in a new era of scientific capability using neutrons as a probe of materials. The SNS, currently under construction at ORNL, will operate at 60 Hz. The possibility of a second target operating at a reduced frequency (5 to 15 Hz) exists and has been studied in detail. Our part in the study of a second SNS target station involves the efficiency of a

* Denotes principal investigator.

pelletized cold moderator. Solid methane moderator lifetimes of the order of hours are estimated for the SNS second target station. One solution to the short lifetime is to use a moderator consisting of solid methane pellets embedded in flowing liquid hydrogen. We have studied the neutron leakage characteristics of a pelletized moderator using the neutron transport code MCNP.

Performance of Neutron Supermirrors

B. J. Heuser,* H. Ju

Innovations in Nuclear Engineering Infrastructure in Education (INIE), U.S. Department of Energy

Neutron supermirrors are optical devices based on total external reflection that allow low energy neutrons to be transported over tens of meters without significant loss. All solids and liquids with sufficient surface smoothness will total-reflect neutrons below a certain critical angle. The critical angle is increased when metal bilayers are deposited. Such multilayer film architectures are called supermirrors. We are currently characterizing Ni-Ti multilayer depositions that have been exposed to high-energy neutron and gamma fluence levels expected for SNS neutron guide sections. The most important measurement technique is neutron reflectivity, since this gives the performance of the supermirror depositions directly. However, we are also characterizing the depositions with x-ray diffraction to measure possible changes in crystallite size. In addition, numerical simulations of interfacial mixing induced by radiation damage are being performed.

Evidence of Superconductivity in Cycled Palladium Hydride and Deuteride Samples (Pd/PdO:H_x and Pd/PdO:D_x)

A. G. Lipson, G. H. Miley*

University of Illinois; New York Community Trust

Electrochemically cycled specially prepared palladium samples (Pd/PdO loaded and deloaded with hydrogen and deuterium) have been studied with thermal desorption and SQUID magnetic measurements. The cycling of the samples produced a high concentration of dislocations, which trap hydrogen and deuterium. An activation energy of 0.91 eV is estimated for deuterium trapped in these dislocations. DC magnetic measurements as well as AC susceptibility studies suggest the presence of weakly diamagnetic state in Pd samples enriched with hydrogen and deuterium. Some samples show signatures of antiferromagnetism at temperatures below 100 K and at low magnetic fields. The material exhibits ferroelasticity that is ascribed to the presence of domains similar to some high-temperature superconductor ceramics. There is a

transition to weak diamagnetism at about 50 K in some samples at fields lower than 1 Oe. Imaginary susceptibility shows the presence of a transition, possibly a new phase that is ascribed to a diamagnetic nanocomposite phase. Further study of this new phase and its properties are under way.

Durability of Advanced Materials

H. Sehitoglu* (Mech. & Indus. Engr.), F. V. Lawrence, Jr.* (Civil & Environ. Engr.), D. F. Socie* (Mech. & Indus. Engr.), J. F. Stubbins,* K. J. Hsia* (Theoret. & Appl. Mech.), N. Chen, H. Hsieh, S. Andrews, T. McGreevy

Fracture Control Program

Recent developments in processing technology have resulted in advanced materials with lower fabrication costs and improvements in microstructural uniformity. To utilize the full potential of these materials, new design tools have to be developed in collaboration with industry. Examples of such materials include metal matrix composites and short reinforcement fibers in epoxy matrices. The metal matrix composites with higher elastic modulus, higher temperature capabilities, and lower weight compared to their counterparts represent excellent opportunities for engine, brake, and rotating components in the ground vehicle industry.

Fatigue Crack Growth and Crack Closure

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Fracture Control Program

The aim of this study is to develop a life prediction methodology for fatigue crack growth based on the changes in crack opening levels with maximum stress level, crack length, geometry, mean stress, and microstructure. The primary tool for the determination of opening stress is an elastic-plastic finite-element simulation of fatigue crack growth. Stress-strain behavior in the model accounts for slip at the microlevel as well as elastic anisotropy. Fatigue crack growth data obtained under conditions of intermediate- and large-scale yielding, including low-cycle fatigue and biaxial loading, are successfully correlated only when closure-modified parameters are employed.

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Fatigue of Welds and Adhesive Joints

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Fracture Control Program

Factors that control the fatigue behavior of welded components are being studied. Analytical methods for estimating the total fatigue life of butt and fillet welds subjected to variable-amplitude loading histories are evaluated. Surface treatments, such as shot peening and laser dressing of the weld toe, are investigated as possible methods for improving the fatigue strength. A new model for estimating the fatigue life of weldments has been proposed for butt, T-joint, and cruciform weldments using the concepts of "crack closure" for cracks emanating from a notch. Results compare favorably with experimental data in the University of Illinois at Urbana-Champaign fatigue data bank and with experimental work in the literature.

Life Prediction Methods for Notched Members under Nonproportional Multiaxial Fatigue

H. Sehitoglu* (Mech. & Indus. Engr.), F. V. Lawrence, Jr.* (Civil & Environ. Engr.), D. E. Socie* (Mech. & Indus. Engr.), J. F. Stubbins,* K. J. Hsia* (Theoret. & Appl. Mech.), N. Chen, H. Hsieh, S. Andrews, T. McGreevy

Fracture Control Program

To develop fatigue life prediction methods for notched components subjected to nonproportional multiaxial fatigue, the local stresses and strains must be related to the global stresses and strains by some approximation procedure, such as Neuber's rule. Experimental tests on notched shafts subjected to proportional and nonproportional loading in tension and torsion are being performed. The results are being used to develop and verify the approximation procedure. Fatigue life estimates will then be made using an appropriate damage model that is based upon observations made during the tests. A life prediction scheme will be developed from the approximation procedure and the appropriate damage model, and this scheme will be verified from the results of the tests.

Probabilistic Methods

H. Sehitoglu* (Mech. & Indus. Engr.), F. V. Lawrence, Jr.* (Civil & Environ. Engr.), D. F. Socie* (Mech. & Indus. Engr.), J. F. Stubbins,* K. J. Hsia* (Theoret. & Appl. Mech.), N. Chen, H. Hsieh, S. Andrews, T. McGreevy

Fracture Control Program

A comprehensive fatigue damage model is being developed to address the following: What governs the nucleation of a microcrack within a single grain or other suitable microstructural unit cell? What governs the growth of this microcrack into adjacent microstructural unit cells? When does the microcrack develop enough plasticity to sustain its growth? These elements will be combined into a model for the entire fatigue damage process.

Copper and Copper Alloys for Fusion Applications

J. F. Stubbins,* M. Li; B. N. Singh,
(Risø National Laboratory)

OMG America; Brush Wellman; Risø Natl. Lab, Denmark; University of Illinois

This research project is aimed at developing an understanding of the performance of copper and copper alloys for fabrication of high heat flux components in nuclear fusion applications. Service performance will be based on irradiation damage behavior and elevated temperature mechanical properties. These features are being examined by testing alloys that have been subjected to high fluences neutron exposure in reactor and performing room and elevated temperature mechanical properties testing.

Fuel Performance in High Temperature Gas-Cooled Reactor for Nuclear Waste Burn-up

J. F. Stubbins*, T. Patten, B. Ye, D. Yun

US Department of Energy; Penn State University, DOE PU2406-UI-4423

This research program addresses major issues regarding the use of high temperature graphite-moderated reactors to burn nuclear waste. The program concentrates on the fuel performance loaded with transuranic actinides and fission products to transmute them to less harmful forms. The program uses computational techniques including MCNP, ORIGEN, and MONTEBURNS. This work is extended to the design of more compact research reactors for possible testing of high burn-up nuclear fuels.

* Denotes principal investigator.

Impedance Spectroscopy as a Feasible Method for Measuring Lead-Bismuth Corrosion

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Los Alamos National Laboratory; U.S. Department of Energy, DOE 57384-001-02-8Y

This impedance spectroscopy (IS) technique employs alternating electric currents of various frequencies to measure the electrical impedance of a surface undergoing corrosion. The IS response can be interpreted to ascertain corrosion rates, corrosion film thickness, and possibly corrosion film type. This technique is being developed to study and monitor corrosion of structural materials in lead-bismuth systems. The work is in collaboration with ongoing lead-bismuth corrosion research at the DELTA-Loop at the LANSCE facility at Los Alamos National Laboratory.

Real-time Corrosion Monitoring in Lead and Lead-Bismuth Systems

J. F. Stubbins*, A. M. Bolind, X. Chen
US Department of Energy, DE-FC07-051D14667

This research program addresses major corrosion issues with the use of lead and lead-bismuth liquid metals for working fluids in the Gen IV LFR concepts and in AFCI accelerator concepts. The work will use Impedance Spectroscopy (IS) corrosion monitoring techniques to measure the kinetics and thermodynamics of the formation of oxides films on reactor structural materials. The IS technology has the major advantage that it can measure the oxide film formation in real time, and is sufficiently compact that it can be deployed at numerous locations in an operating system to monitor local corrosion processes directly.

The Effect of H and He on Irradiation Performance of Fe and Ferritic Alloys

J. F. Stubbins*, M. A. Okuniewski, C. Tomchik, X. Pan
US Department of Energy, DE-FC07-051D14665

This research program addresses radiation damage and effects issues in advanced reactor and accelerator driven systems. The experimental program examines the evolution of point defects and defect structures as a function of irradiation exposure (dpa), irradiation temperature, and H and He production (appm H/dpa and appm He/dpa) in single crystal Fe, polycrystalline Fe, binary and ternary Fe alloys and advanced ferritic/martensitic steels. The modeling work examines defect and defect structure survivability with and without the influences of H and He during irradiation by use of molecular dynamics (MD) simulations. These results are used to examine the longer-time scale evolution of

extended defect structures using kinetic Monte Carlo (KMC) simulations.

The Effect of Localized Flow on Fracture of Reactor Components

J. F. Stubbins,* X. Pan, X. Wu
U.S. Department of Energy, DOE DEFG07-02ID14337

Most reactor components are designed to resist brittle fracture by plastic deformation. However, brittle fracture can occur when structural material cannot undergo general plastic deformation due to the effects of radiation exposure through a process referred to as flow localization or local plastic instability. This process results in a fracture mode that appears to be brittle since only small volumes of the material are able to deform through plastic flow. This study addresses the conditions under which plastic flow localizes to cause embrittlement; it models the deformation process so that relevant material constitutive equations can be used in finite element structural analysis; and it characterizes the damaged microstructure associated with flow localization.

Radiation Damage in Borosilicate Glass

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Nuclear Engineering Education Research (NEER), U.S. Department of Energy, DF-FG07-01ID14121

The storage of long-lived radioactive actinide isotopes, generated during the consumption of uranium-based commercial nuclear reactor fuel, is an important societal issue in the United States. Two media that have received significant research interest are ceramics and glass. The goal of our project is to better understand the response of borosilicate glass as a nuclear waste storage medium. As part of a fundamental investigation into the response of borosilicate glass, we have performed small angle x-ray scattering measurements of He-implanted samples. These results allow us to correlate the onset of He bubble formation to the local concentration to determine the solubility limit. In addition, the effect of He bubble stability under heavy ion bombardment has been investigated.

Nuclear Power, Operations, and Control

Characteristics of International Research Reactors

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U.S. Department of Energy, DOE-ANL 2F-02022

A detailed collection of research reactor characteristics was assembled, including thermal performance, physical

* Denotes principal investigator.

configurations, and capabilities for supporting nuclear research and development of next-generation university research reactors.

Development of Advanced Direct Perception Displays for Nuclear Research Reactors (with Applications to Advanced Control Systems for Nuclear Power Plants) to Enhance Monitoring, Control, and Fault Management

B. G. Jones*

U.S. Department of Energy, DOE PU 2406-UI-4423; University of Illinois

A direct perception interface (DPI) integrates information into a unified animated diagram that supports fault diagnosis more strongly than conventional displays. Building on earlier work on a DPI for nuclear thermal hydraulics, this project will lead to a complete suite of DPI displays for an entire nuclear reactor plant, from nucleonics to power generation. It will also take into account the need for teams of operators to extract different types of information from a DPI. A special case of reactor start-up has been examined that demonstrates the effectiveness of the display. The initial application to university research reactors will enable field-testing of the concepts.

Innovations and Enhancements for a Consortium of Big-10 University Research and Training Reactors

J. F. Stubbins,* B. Heuser,* R. Uddin,* B. G. Jones,* Y. Gu, T. Patten, G. Danagoulian, S. Singh, F. Teruel, F. Wang, Y. Yan, D. Yun, B. Ye, J. Hu, S. Markidis
U.S. Department of Energy; Penn State University, DOE PU 2406-UI-4423

A consortium of six Big-10 universities (University of Illinois, Ohio State University, University of Michigan, Penn State University, Purdue University, and University of Wisconsin) are working to develop and grow university research and training reactors research and outreach as well as next-generation university research and training reactors (URTR) design in the United States. This multiyear program has four major objectives: to develop innovative programs in graduate research and undergraduate education and training that utilize experimental URTR facilities; to develop and design a "virtual" URTR for use in education and research with the intention of constructing a new URTR; to create a novel educational outreach and education program for the nuclear industry, the DOE laboratories, and other regional educational institutions at all levels; and to develop a multidisciplinary, multi-university research grant program to enable collaborative research between the four consortium university programs,

other schools and colleges, and industrial and laboratory partners.

Flashing Instability for Next-Generation Natural Circulation Reactors

R. Uddin,* Q. Zhou

U.S. Department of Energy, DE-FG07-00ID13923

Simulation of flashing in unheated risers of natural circulation based reactor designs requires a new development of the basic set of thermal hydraulic equations that allow the saturation enthalpy to vary with pressure (and hence elevation). We have developed such a model to study the stability and dynamics of reactors susceptible to flashing. In the first phase, a thermal hydraulic model was developed to simulate the flashing phenomenon. This was then extended to coupled neutronics-thermal hydraulics simulation. Parametric dependence of the coupled phenomenon has been investigated. Based on results obtained here, an explanation is provided for the discrepancy between data and simulation results.

New Research Reactor Designs

R. Uddin, F. Teruel, J. Hu

U.S. Department of Energy, Penn State University, DOE PSU 2406-UI-4423

Research reactors have played an important role in the development of nuclear power as well as in fundamental research in science and engineering. New constraints have been placed on their design due to safety and security considerations. A design is usually dictated by the desired flux level, spectrum, core life, and irradiation facilities. We are exploring design ideas that will allow maximum utility of a future research reactor within the new constraints. New designs have been proposed and modeled.

Nuclear Engineering Applications Using CFD Codes

R. Uddin,* D. Rock

Argonne National Laboratory

Significant safety margins are imposed on reactor operations because computer codes used to design and simulate these systems are often based on "lumped" analyses. A public domain CFD code is likely to help increase the use of CFD by nuclear engineers. We are working on adapting the CHAD code, developed at LANL, for general purpose CFD simulations of nuclear engineering applications. Specific tasks include: speed up of the solution of the continuity equation using the tools for the PETSc solver; review of the treatment of certain boundary cells; and demonstration of the capability of the code by solving practical nuclear engineering problems.

* Denotes principal investigator.

Virtual Models of GEN-IV Reactors

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Y. Yan

U.S. Department of Energy, DE-FG07-03ID14501

We are combining developments in virtual reality technology with the 30-year experience of operating GEN-II reactors to achieve better efficiency for GEN-IV nuclear reactor designs. A framework is being created to model and then test GEN-IV designs in virtual environment vis-à-vis refueling operations, repair operations, and operator training, and to allow better planning of regular maintenance operations. Different options for the refueling experience can be tested in a virtual environment for safety and to minimize exposure and refueling time. By altering the plant layout in the virtual environment, for example, the refueling time can be minimized. Similarly, critical components of the layout can also be examined in a virtual environment to ensure that repair or replacement can process in a minimum amount of time. The most obvious benefit of a virtual model will be the operator training that may lead to reduced unintended downtime for GEN-IV reactors. Recent developments include display of the radiation field in the virtual environment.

Reactor Physics and Reactor Kinetics

Construction of Exact Difference Equations with Lie Groups and Gauge Functions

R. A. Axford,* T. J. Grove

University of Illinois; Los Alamos National Laboratory

New methods are developed to construct exact difference equations from which numerical solutions of both initial value problems and two-point boundary value problems involving first- and second-order ordinary differential equations can be computed. These methods are based upon the transformation theory of differential equations and require the identification of symmetry properties of the differential equations. The concept of divergence-invariance of a variational principle is applied to the construction of difference equations. It is shown how first- and second-order ordinary differential equations that admit groups of point transformations can be integrated numerically by constructing exact difference equations.

Lie Group Symmetries and Difference Equations

R. A. Axford,* K. Li

Los Alamos National Laboratory

Two methods have been developed to obtain exact numerical solutions of second-order differential equations. These are based upon the concept of divergent-invariant

variational principles and the concept of differential-difference invariants. In the first method, the symmetry properties of a variational principle yield first-order conservation laws that are discredited to produce superconvergent numerical solutions. In the second method the symmetry properties of second order differential equations lead to differential-difference invariants with which difference equations with zero truncation error can be constructed. It has been demonstrated that exact eigenvalue spectra are obtained.

Stochastic Neutronics

R. A. Axford*

Los Alamos National Laboratory

The time evolution of the neutron population in a fissile assembly containing an insufficiently large enough number of neutrons to be able to define a probable number of neutrons per unit volume of phase space must be analyzed on the basis of stochastic formulations. New methods for obtaining the generating functions from which dynamics parameters and neutron fluctuations can be found have been developed. Methods for multidimensional assemblies are being studied.

Design of Small-Angle Neutron Scattering (SANS) Instrument at the Indiana University Low-Energy Neutron Source (LENS) Facility

B. J. Heuser,* G. Danagoulian,

W. M. Snow (Indiana Univ.), D. Baxter (Indiana Univ.)

National Science Foundation

The NISP neutron simulation package from Los Alamos National Laboratory is being used to optimize the first generation SANS instrument at the Indiana University Low-Energy Neutron Source (LENS) Facility. This facility will generate neutrons from the Be(p, n) reaction and will have a solid methane cold source. Our design effort has the goal of determining the optimized instrument configuration. This work has identified two optimum configurations easily accessible within the operational parameters of the instrument.

Perturbation Theory of Neutron Spin Interactions with Time-Dependent Magnetic Fields

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W. M. Snow (Indiana Univ.), D. Baxter (Indiana Univ.)

Indiana University

Neutron resonance spin echo (NRSE) techniques result in excellent energy resolution without the long, constant-B fields required for neutron spin echo. We are investigating the use of NRSE for small-angle neutron scattering. Our treatment of the problem involves the application of

* Denotes principal investigator.

quantum mechanical perturbation theory to investigate the effect of beam divergence, magnetic field tilt, and a finite neutron pulse width. It is anticipated that these results will guide the development of a new instrument at the Indiana University Cyclotron Low Energy Neutron Source.

Virtual Nuclear Reactor Project at the University of Illinois at Urbana-Champaign; Coupling of Monte Carlo Code for Neutron and Photon Transport (MCNP) and Neutron Scattering Instrument Performance in a Virtual Environment

B. J. Heuser,* G. Selvaggi

Innovations in Nuclear Engineering Infrastructure in Education (INIE), U.S. Department of Energy, DOE PU 2406-UI-4423

The virtual reactor project at the University of Illinois is envisioned as a teaching and research opportunity in which a nuclear research reactor will be “constructed” and then operated in real time. As part of this project, we are bringing together two neutron transport codes, Monte Carlo Code for Neutron and Photon Transport (MCNP) and Neutron Instrument Simulation Package (NISP), in a virtual environment. The overall goal of the project is to visualize neutron production in the core and to couple this production to neutron absorption in fissile isotopes via MCNP. In addition, fuel temperature variation, coolant flow, and coolant temperature variation will be determined with heat and mass transfer numerical simulation codes. Neutron moderation and transport beyond the core into the reflector and eventually into beam tubes will also be tracked, with the objective of providing a virtual source for neutron scattering.

A RELAP-Based Reactor Simulator

R. Uddin,* K. D. Kim

Innovations in Nuclear Education and Infrastructure (INIE) Program, U.S. Department of Energy; DOE PSU 2406-UI-4423

Taking advantage of the user-friendly graphical output of Labview and its capability to broadcast these results over the World Wide Web, the widely used nuclear reactor safety code has been modified so that its output is available in Labview based GUIs. The output is available not only on the local machine but also, when broadcasted, on any machine with an Internet browser and Labview runtime engine installed.

Space Propulsion and Power Systems

Dense Plasma Focus (DPF) Propulsion

G. H. Miley,* Y. Yang, R. Thomas

U.S. Air Force

Use of a dense plasma focus (DPF) for advanced space propulsion applications is under evaluation. The current research focuses on achieving aneutronic fusion using advanced fuels such as D-He3 or p-B11. The DPF is uniquely suited for such operations due to its ability to obtain a high ion/electron temperature ratio. Methods of achieving suitable burn conditions with a minimal increase in ignition temperature are being explored along with ways of reflecting Bremsstrahlung back into the core of DPF fusion exhaust. Ways for achieving the DPF pinch for use in air breathing systems, along with methods for efficient electrical power extraction and recirculation to the DPF, are under consideration.

Fuel Cell Systems Analysis for Space Applications

G. H. Miley,* R. Gimlin, R. Burton

N.Y. Trust; NASA

A systems study and generalized parameterization of a direct hydrogen peroxide/sodium borohydride fuel cell is presented. Of specific interest are those applications suited for modern and next-generation spacecraft. First, a thorough study of a similar fuel cell and other related projects will be presented, with the goal of identifying future avenues of study to optimize the University of Illinois’ fuel cell. Next, a generalized parameterization of Illinois’ hydrogen peroxide/sodium borohydride fuel cell will be carried out, with a strong emphasis on specific mass and power densities. Two spacecraft power scenarios are then addressed using this generalized parameterization. Last, the electrical and thermal subsystems for satellites will be discussed, with a key emphasis placed on how Illinois’ fuel cell will interact with the spacecraft. The purpose of this project is not to define the design of Illinois’ hydrogen peroxide/sodium borohydride fuel cell, but instead to present potential design options.

Laser Ablation of a Micro Laser Plasma Thruster

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This work involves the experimental study of laser ablation physics. The goal of the work is to gain an understanding of the physics of plasma formation and expansion due to laser ablation. Research has been done on low power, long pulse, laser generated plasmas, applicable to current and

* Denotes principal investigator.

next-generation propulsion mechanisms for Air Force satellites. A 920nm laser heats a target material of Polyvinyl Chloride (PVC) or Glycidyl Azide Polymer (GAP) after passing through a transparent substrate. The substrate acts to protect the laser optics from coating of target material. Once heated, the target material boils off the surface and transforms into a vapor phase that generates thrust. The discharge occurs on the order of a couple of milliseconds. The goal of this propulsion unit is to enable higher values of Isp while keeping the overall propulsion system weight low. With the success of this propulsion unit, the Air Force can employ the development of nano- and pico-weight class satellites.

Research on a Unique Regenerative Hydrogen Peroxide Based Fuel Cell

G. H. Miley,* N. Luo*

Defense Advanced Research Projects Agency; NPL Associates, Inc.

Development of a unique peroxide-based fuel cell using liquid phase hydrogen peroxide (H_2O_2) directly in its cathode is under study. This cell provides an alternative to traditional fuel cells that employ gaseous oxygen, providing an ideal surface power for human exploration of the moon and Mars. It offers some important benefits compared to traditional fuel cells and batteries, including: very high (theoretical) energy density of over 2500 watt-hr/kg; safe, long-term stable storage of the energetic fuel, which enables lunar and Martian surface exploration of months and longer; very high efficiency (over 80%) through use of H_2O_2 , which overcomes the oxygen over-potential problem inherent to prior fuel cell designs; simple construction with a unitized regenerative operation employing the electrochemical pair $NaBH_4/H_2O_2$; a closed-cycle (regeneration) performance twice that of the best lithium-ion batteries. Operation of a watt-level cell has been successfully demonstrated at the University of Illinois at Urbana-Champaign.

Spherical Inertial Electrostatic Confinement (IEC) Jet Thruster Studies

G. H. Miley,* Y. Yang, J. Webber, H. Momota

National Aeronautics and Space Administration (NASA) NAS8-0003; NPL Associates, Inc.

Experimental and theoretical studies are being performed on the spherical inertial electrostatic confinement (IEC) jet thruster to better understand its plasma physics behavior and performance characteristics. The goal is to optimize the jet design and operational conditions for use as a 500 to 800 W spacecraft thruster. The IEC jet thruster creates and accelerates ions toward a central spot, which then

escape out through a single quasi-neutral plasma jet, creating thrust. Faraday cup and thermocouple measurements are being taken to determine particle energy distributions and heating power of the jet, and hence, the device thrust and efficiency.

Technical Assistance to NPL on NASA Phase II Project: "A Breakthrough Fusion Power Unit for Space Applications"

G. H. Miley*

National Aeronautics and Space Administration (NASA), NPL SRA00-239

This project is carried out in the Fusion Studies Lab (FSL) in the Department of Nuclear, Plasma and Radiological Engineering. In order to build a new reactor design for power or thrust applications, a breakeven, $Q \geq 1$, prototype will first be demonstrated. The primary objectives of this Phase II project are to investigate the fundamental physics issues associated with inertial-electrostatic confinement as a new breakeven reactor concept and to demonstrate the feasibility of an IEC reactor to reach breakeven. Such a demonstration will satisfy all the physics questions associated with breakeven operation and will identify the salient engineering issues for the final order of magnitude scale-up necessary for future stages.

Thermal Hydraulics and Reactor Safety

Similarity Analysis and Invariant Difference Schemes for Hydrodynamics, Transient Heat Conduction Plasma Physics, and Multigroup Neutronics

R. A. Axford,* T. J. Grove

University of Illinois

Concepts from the transformation theory of ordinary and partial differential equations have been applied to determine self-similar solutions of the nonlinear partial differential equations of nonlinear and linear diffusion phenomena, hydrodynamics, and plasma physics. An invariant source iteration method for one- and two-dimensional multigroup neutronics calculations has been developed. Exact difference equations for transient heat conduction have been determined. The theory of Lie group extensions in discretized jet spaces needed to construct invariant difference schemes has been worked out in terms of grid point values of dependent variables.

* Denotes principal investigator.

Boiler Waterwall Deposition Model Development Support

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Research is under way on the initial development of an aggregate model to predict the inception and growth of deposition activity in fossil boiler tubes and the subsequent related degradation of thermal performance with deposition layer growth. Suspended particulate and corrosion products are believed to be primary contributors to the buildup of the observed porous layer.

Phenomenological models are being developed that incorporate bubble nucleation, particulate charge, interfacial surface charge, energy transfer, and solute/particle concentration distributions. The porosity of the porous layer and its chimney structure are coupled with surface tension to provide the driving wicking mechanism for multiphase flow within the layer and the surprisingly high capacity to transfer energy through it. Estimates of the limiting performance and tube failure will be made for variations in deposition layer thickness, porosity, and composition for varying thermal conditions. The results will support both boiler design and unit operations and management of fossil power plants.

Effect of Boiling on Interfacial Behavior during Melt Quench Processes

B. G. Jones*

U.S. Department of Energy, DEFG07-89ER12900

In conjunction with the Department of Mechanical and Industrial Engineering

The effects of interfacial mixing and contact area between two liquids of differing densities and temperatures have been studied, utilizing a high-density, high-temperature liquid jet column passing through a lower density, low-temperature liquid pool. Heat transfer effects, including the effects of vapor generation of pool fluid as well as jet break-up and solidification, are modeled. Analytical modeling was carried out at the University of Illinois at Urbana-Champaign, while simulant experimental studies of both single- and multiple-injected columns were conducted at Argonne National Laboratory. Good agreement between model predictions and experimental data is found.

Hypervapotron Isothermal Flow Resistance Tests for Use in ITER Divertor Cooling

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D. Driemeyer* (McDonnell Douglas-St. Louis)

U.S. Department of Energy, DE-YBE233R-C04A

Isothermal flow tests have been conducted to determine parametric flow resistance characteristics of hypervapotron (i.e., boiling in single-sided, ribbed-flow channels) configurations using low-pressure water systems, with prototypic dimensions and flow rates. Experimental data indicate friction factors are significantly lower than previously published correlations and are only slightly higher than smooth wall values. For small flow channel height, of the dimension of the tooth pitch or smaller, the tests show friction factor increases, which are increasingly sensitive to decreasing channel height dimensions.

Hypervapotron Thermal Performance Tests of Boiling Heat Transfer using Simulant Fluid (Freon 134a) with Application for ITER Divertor Cooling

B. G. Jones,* P. Chen, W. Wu

University of Illinois Research Board

In cooperation with the Department of Mechanical and Industrial Engineering

Using reduced-pressure thermodynamic characterization with simulant fluids, thermal performance tests have been conducted to determine boiling heat transfer characteristics of hypervapotron configurations (i.e., boiling in single-sided, ribbed-flow channels) using a Freon loop system, with prototypic dimensions and flow rates. Performance in boiling smooth single-sided channels is being conducted in parallel under identical flow and heat flux ranges. Initial experimental data exhibits hypervapotron configuration boiling performance that exceeds that of smooth surfaces, including critical heat flux conditions.

Measurement and Analysis of Bubble Behavior in Subcooled Boiling Flows

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University of Illinois; U.S. Department of Energy, 493661/DOE

In cooperation with the Department of Mechanical and Industrial Engineering

This research examines bubble behavior under subcooled nucleate flow boiling conditions, using a high fidelity digital imaging apparatus. Refrigerant R-134a is chosen as a simulant fluid due to its merits of having smaller surface tension, reduced latent heat, and lower saturation

* Denotes principal investigator.

temperature than water. Boiling curves are measured with varying experimental parameters, e.g. pressure, inlet subcooled level, flow rate, and so forth. Images at frame rates up to 2000/s are obtained, showing characteristics of bubble behavior under a range of conditions. Bubble size and position information are calculated via Canny's algorithm for edge detection and Fitzgibbon's algorithm for ellipse fitting. Results compare well with other published data.

Modeling and Thermal Performance Evaluation of Subcooled Nucleate Boiling Effects on Formation of Porous Crud Layers on Fuel Pin Surfaces Leading to Axial Offset Anomaly in PWR Cores

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U.S. Department of Energy, DE-FG07-00ID13924

In conjunction with the Department of Mechanical and Industrial Engineering

A study of axial offset anomaly (AOA) conditions with PWR cores, focusing on boron holdup and retention in porous layers on fuel pins, is being conducted. Computational models indicate sufficient boron accumulation in solution within the crud layer could account for the observed axial power shift. Parameterization over the range of the geometric characteristics of the crud suggests that precipitation of boron from solution is possible. Examination of potential mechanisms for crud deposition, including radiochemical processes, suggests that combined effects of electrolysis of water in the core may contribute to formation and help explain controlling mechanisms. The research focus is on clarifying which physical mechanisms dominate the processes. The nuclear power industry strongly desires clarification and resolution of this issue.

Modeling of Particulate Deposition Processes Under Subcooled Nucleate Boiling Conditions

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To understand the deposition process and predict the deposition rate during subcooled nucleate boiling is the main goal of this study. The micro-layer evaporation model (MEM) is widely used to explain the deposition process in saturated boiling situation. However, the bubble dynamics for subcooled boiling and saturated boiling are different. In this paper, two other kinds of deposition mechanisms, besides MEM, are studied. They are Marangoni effect due to surface tension gradients, and particle-bubble interaction due to the hydrophobic nature of particles. Both

of them can change the particle transport coefficient and impact the deposition rate. A preliminary model is proposed to include these three mechanisms. If the Marangoni flow and particle-bubble interaction are proved to be the important deposition mechanisms in subcooled boiling, some possibilities will be proposed to mitigate the deposition.

Subcooled Nucleate Boiling Effects on Formation of Porous Crud Layers on Fuel Pin Surfaces Leading to Axial Offset Anomaly in PWR Cores and Modeling and Thermal Performance Evaluation of Such Layers

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In conjunction with the Department of Mechanical and Industrial Engineering

A study of axial offset anomaly (AOA) conditions with PWR cores, focusing on boron holdup and retention in porous layers on fuel pins, is being conducted. Computational models indicate sufficient boron accumulation in the solution in the crud layer could account for the observed axial power shift. Parameterization over the range of the geometric characteristics of the crud suggests that precipitation of boron from solution is likely. Examination of potential mechanisms for crud deposition, including radiochemical processes, suggests that combined effects of electrolysis of water in the core may contribute to formation and help explain controlling mechanisms. The research focus is on clarifying which physical mechanisms dominate the processes. The nuclear power industry strongly desires clarification and resolution of this issue.

Understanding Local Concentration Levels of ^{10}B and Radiolysis Products (H_2 , O_2 , and H_2O_2) within the Porous Crud Layer

B. G. Jones, H.-J. Joe
University of Illinois; U.S. Department of Energy, DE-FG07-00ID13924

An understanding of local concentration values of radiolysis products in the porous crud layer may provide insight into conditions leading to corrosion and crud deposits on the fuel pin clad surface. This research shows that an understanding of local concentration levels of B^{10} and radiolysis products (H_2 , O_2 , and H_2O_2) within the porous crud layer may play an important role leading to crud growth on the fuel pin clad and on its relation to axial offset anomaly (AOA), or crud induced power shift (CIPS). Boron holdup is established in the crud and results in a very large boron mass within the crud layer, due to coolant

* Denotes principal investigator.

evaporation at depth in the crud, adsorption, and possibly Bonaccordite (Ni_2FeBO_5) formation. High $\text{B}^{10}(\text{n}, \alpha) \text{Li}^7$ reaction rates cause an increase of water decomposition by energetic α -particle radiolysis within the crud layer. Thus, 10B removal by this transmutation reaction reduces the 10B fraction in the bulk coolant. After the crud layer on Zircaloy fuel cladding reaches a threshold thickness, the subsequent oxidation rate is possibly restricted by water radiolysis in oxide cracks and pores. Therefore, radiolysis within this thick porous oxide (or crud) is independent of the water chemistry in the bulk coolant. It is dominated by highly localized water chemistry near the metal-oxide interface. This is supported by our Monte Carlo simulation calculations of local H_2 and O_2 concentrations, which are directly related to oxidation processes within the crud layer. The H_2 species dominates in the upper portion, about the upper 10 to 20 percent, of the thick porous crud region. The local concentration distribution of O_2 , governed by molecular diffusion, however, shows the opposite behavior of H_2 .

Visualization of Subcooled Flow Boiling in Hypervapotron Configuration for Cooling of Proton Accelerator Beryllium Target

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University of Illinois; Indiana University (SBC IN DMR-0220560-NSF Prime); University of Illinois at Urbana-Champaign Research Board; Department of Nuclear, Plasma and Radiological Engineering

In conjunction with the Department of Mechanical and Industrial Engineering

This work reports on experimental and design studies that examine the subcooled boiling on the enhanced heat transfer surface of the hypervapotron structure as applied to cooling a Beryllium target in an intense proton accelerator beam. The laboratory experiment is conducted for steady state, subcooled boiling with simulant fluid Freon (R134A) with heat fluxes, ranging from 50 to 800 kW/m^2 . In the application, the Beryllium target application is subjected to a pulsed proton beam and water-cooled with steady state heat flux levels up to 6 MW/m^2 . Transient driven thermal stress-strain levels are estimated using ANSYS software to ensure that the operating conditions are within allowable limits to avoid target failure from stress levels exceeding elastic limits and from cycling by the pulsed thermal source.

A Study in Heat and Mass Transfer with Boiling in Porous Deposits

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University of Illinois

In conjunction with the Department of Mechanical and Industrial Engineering

A numerical/analytical model of boiling heat transfer in heterogeneous porous layers with and without chimneys has been conducted. Experimental observations from the literature and in laboratory observations have provided qualitative modeling information and model refinements. The 1-D and 2-D models have been evaluated numerically with nonlinear coupling between mass, momentum, energy, capillary pressure, and evaporation rate. Good agreement with published data has been obtained. Examination of artificially created layer performance suggests broad potential application for controlled boiling heat transfer, such as computer chip cooling via Freon or other CFCs, with heat fluxes in excess of 100 W/cm^2 , and in steam generator tube performance. Variable porosity layers are being formulated to reflect observed crud characteristics.

BWR Stability and Bifurcation Analysis Using a Novel Reduced Order Model

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Systems Behavior, Paul Scherrer Inst., Switzerland,
and Swiss Fed. Inst. of Tech. (EPFL)]
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A novel analytical, reduced order model has been developed to simulate different types of instabilities encountered in heated channels and BWRs, namely, density wave oscillations (DWOs), as well as in-phase and out-of-phase oscillations in the reactor core. The complete two-parallel channel model comprises three main parts: spatial lambda-mode neutron kinetics with the fundamental and first azimuthal modes, fuel heat conduction dynamics, and core thermal-hydraulics based on a drift flux model representation of the two-phase flow. The thermal-hydraulic part of the model is validated against experimental data and compared with several models developed earlier.

* Denotes principal investigator.

CFD Simulation of the International Reactor Innovative and Secure (IRIS) Reactor Design

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INIE-U.S. Department of Energy; DOE PSU 2406-UI-4423

CFD has been identified as a key new technology toward the development of a next-generation research reactor. In that regard, experience with current use of CFD to address thermal-hydraulics issues arising in the design of power reactors is very useful. Pressurized, light water-cooled, medium-power (1000 MWt) IRIS (International Reactor Innovative and Secure) nuclear reactor has been under development for three years by an international consortium of over twenty organizations from nine countries. The development of a new nuclear plant concept presents the opportunity and potential for significant use of computational fluid dynamics (CFD) in the design process. A group of scientists from several countries has been given the mission of investigating the many application opportunities for CFD. The key point is to improve the use of CFD as a design tool for virtual tests in order to simplify the optimization effort for the nuclear plant's components. We are participating in solving CFD problems that require very-large-scale parallel computing capabilities.

Safety and Stability of Supercritical Water Reactor

R. Uddin,* P. Jain

University of Illinois

A supercritical water reactor will experience density change inside the core similar to that experienced in BWRs. Hence, concerns related to stable operation of BWRs, such as nuclear coupled density wave oscillations, must be addressed for SCWRs as well. We are developing models to study the safe operations of SCWRs.

Turbulence Model for Porous Media

R. Uddin,* F. Teruel

INIE-U.S. Department of Energy; DOE PSU 2406-UI-4423

Integral analysis of a next-generation research reactor design will likely require porous media approximation to describe flow through the reactor core. Turbulent flow modeling in porous media has begun to receive attention only recently. We are exploring ways to enhance existing porous media k-epsilon as well as LES models to more accurately describe turbulent flow in such media.

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Neumann, M. J., Shin, H., Qiu, H., Ritz, E., DeFrees, R. A., Hendricks, M. R., Alman, D. A., Jurczyk, B. E., Ruzic, D. N., and Bristol, R. **Evaluating advanced fuel candidates in surface cleaning of optics by plasma exposure (scope).** Emerging Lithographic Technologies IX (San Jose, CA, Mar. 2005). Proceedings of the International Society for Optical Engineering—Progress in Biomedical Optics and Imaging 1125-1136 (2005).

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Arms Control, Disarmament, and International Security

Singer, C. E. **Time series calibrated carbon emissions and atmospheric response.** United States Climate Change Science Program Workshop (Arlington, VA, Nov. 2005).

Computational Mechanics

Gu, Y. and Uddin, R. **A hybrid method for multi-group neutron diffusion equations in arbitrary geometry.** International Topical Meeting on Mathematics and Computations, Supercomputing, Reactor Physics and Nuclear and Biological Applications (Avignon, France, Sep. 2005).

Rock, D. T., Uddin, R., and Tzanos, C. P. **Multiple parallel solvers in a CFD code using PETSc.** 2005 Winter Meeting of the American Nuclear Society (Washington, D.C., Nov. 2005). Transactions of the American Nuclear Society 541-542 (2005).

Yan, Y., Sobh, N., and Uddin, R. **Computational fluid dynamics (CFD) simulation of research reactor.** International Topical Meeting on Mathematics and Computations, Supercomputing, Reactor Physics and Nuclear and Biological Applications (Avignon, France, Sep. 2005).

Low-Energy Nuclear Reactions

Lipson, A. G. and Miley, G. H. **A novel portable ferroelectric source of fast MeV neutrons for homeland security applications.** 2005 Winter Meeting of the American Nuclear Society (Washington, D.C., Nov. 2005). Transactions of the American Nuclear Society 329-330 (2005).

Nuclear Engineering Education and Outreach

Gu, Y. and Uddin, R. **Real time, distance lab via labview and webcam.** 2005 Annual Meeting of the American Nuclear Society (San Diego, CA, Jun. 2005). Transactions of the American Nuclear Society 789-790 (2005).

Ramsey, S. D., Rokusek, D. L., Tomchik, C. A., Wu, Y., and Jones, B. G. **Inductively coupled plasma torch for aqueous nuclear waste slurry vaporization.** 2005 Winter Meeting of the American Nuclear Society (Washington, D.C., Nov. 2005). Transactions of the American Nuclear Society 437-438 (2005).

Nuclear Fusion

Wu, L., Miley, G. H., and Momota, H. **Space-charge neutralization of heavy ion beams via electron injection.** Proceedings of the 15th International Symposium on Heavy Intertial Fusion HIF 2004 (Princeton, NJ, Jun. 2004). Nuclear Instruments and Methods in Physics Research, Section A: Accelerators, Spectrometers, Detectors and Associated Equipment 533-537 (2005).

Nuclear Materials, Materials Science and Performance, Radiation Effects, and Waste Management

Miley, G. H., Narne, G., and Woo, T. **Use of combined NAA and SIMS analyses for impurity level isotope detection.** Sixth International Conference on Methods and Applications of Radioanalytical Chemistry (Kailua-Kona, HI, Apr. 2003). Journal of Radioanalytical and Nuclear Chemistry 691-6 (2005).

Wu, X., Pan, X., Li, M., and Stubbins, J. F. **Modeling tensile response and flow localization effects in 316SS after exposure to spallation and fission irradiation environments.** Proceedings of the 6th International Workshop on Spallation Materials Technology IWSMT-6 (Hayama, Kanagawa, Japan, Nov. 2003). Journal of Nuclear Materials 302-307 (2005).

Nuclear Power, Operations, and Control

Griffith, J., Hu, J., Karancevic, N., Teruel, F. E., Yan, Y., Stubbins, J., Uddin, R., and Stubbins, J. F. **Research and virtual reactor design at UIUC, invited.** 2005 Winter Meeting of the American Nuclear Society (Washington, D.C., Nov. 2005). Transactions of the American Nuclear Society 873-875 (2005).

Hu, J., Teruel, F. E., and Uddin, R. **Reactor design efforts at UIUC, invited.** 2005 Annual Meeting of the American Nuclear Society (San Diego, CA, Jun. 2005). Transactions of the American Nuclear Society 154-156 (2005).

Zhou, Q. and Uddin, R. **In-phase and out-of-phase oscillations in BWRs: Impact of azimuthal and asymmetry and second pair of eigenvalues, invited.** 2005 Winter Meeting of the American Nuclear Society (Washington, D.C., Nov. 2005). Transactions of the American Nuclear Society 383-385 (2005).

Zhou, Q. and Uddin, R. **Stability analyses of an integrated neutronics-thermal hydraulics model of natural circulation boiling water reactor (BWR) under low pressure.** International Topical Meeting on Mathematics and Computations, Supercomputing, Reactor Physics and Nuclear and Biological Applications (Avignon, France, Sep. 2005).

Reactor Physics and Reactor Kinetics

Hu, J. and Uddin, R. **A multipurpose research reactor design.** International topical meeting on mathematics and computations, Supercomputing, Reactor Physics and Nuclear and Biological Applications. (Avignon, France, Sep. 2005).

Sugawara, K. and Uddin, R. **Automated conversion of Keno input files to Monte Carlo N-Particle (MCNP) input files and comparison of Keno and Monte Carlo N-Particle (MCNP) results.** American Nuclear Society (LaGrange Park, IL, Apr. 2005).

Teruel, F. and Uddin, R. **An alternative model for neutron flux maximization in research reactors.** International Topical Meeting on Mathematics and Computations, Supercomputing, Reactor Physics and Nuclear and Biological Applications (Avignon, France, Sep. 2005).

Teruel, F., Hu, J., and Uddin, R. **Reactor design efforts at University of Illinois of Urbana-Champaign.** American Nuclear Society (San Diego, CA, Jun. 2005).

Space Propulsion and Power Systems

Luo, N., Miley, G. H., Shrestha, P. J., Gimlin, R., Burton, R., Rusek, J., and Holcomb, F. **H₂O₂-based fuel cells for space power systems.** 3rd International Energy Conversion Engineering Conference (San Francisco, CA, Aug. 2005). Collection of Technical Papers for the 3rd International Energy Conversion Engineering Conference 1947-1967 (2005).

Miley, G. H., Momota, H., Webber, J., Yang, Y., Thomas, R., Takeyama, Y., and Wu, L. **Thruster design for IEC-based spacecraft propulsion.** Proceedings of the American Nuclear Society Embedded Topical Meeting, 2005 Space Nuclear Conference (San Diego, CA, Jun. 2005). American Nuclear Society Embedded Topical Meeting, 2005 Space Nuclear Conference 775-780 (2005).

Thermal Hydraulics and Reactor Safety

Wu, W., Chen, P., Jones, B. G., and Newell, T. A. **A study on bubble growth and bubble movement in horizontal sub-cooled boiling flows.** 2005 Winter Meeting of the American Nuclear Society (Washington, D.C., Nov. 2005). Transactions of the American Nuclear Society 397-398 (2005).

Zhou, Q. and Uddin, R. **Nonlinear dynamics of flashing in a natural circulation loop under low pressure.** 5th International Symposium of Multiphase Flow (Xi'an, China, Jul. 2005).

Zhou, Q. and Uddin, R. **An integrated model of natural circulation loop under low pressure.** 2005 Annual Meeting of the American Nuclear Society (San Diego, CA, Jun. 2005). Transactions of the American Nuclear Society 782-784 (2005).

Awards and Honors

Roy A. Axford

Everitt Award for Teaching Excellence, University of Illinois College of Engineering, 1985
Nuclear Engineering Student's American Nuclear Society Excellence in Undergraduate Teaching Award, University of Illinois, 1990, 1995, 1997, 1999, 2002, 2004
Distinguished Faculty Member, Alpha Nu Sigma, 1991
Graduate College Outstanding Mentor Award, University of Illinois, 2004
Student Award for Excellence in Undergraduate Teaching, University of Illinois, 2004

Daniel E. Hang, Emeritus

Honorary Member, Alpha Nu Sigma
Life Senior Member, Institute of Electrical and Electronics Engineers
Life Member, Illinois Society of Professional Engineers
Life Member, National Society of Professional Engineers
Stanley H. Pierce Award, University of Illinois College of Engineering, 1981
Distinguished Service Award, Central Zone of National Council of Examiners for Engineering and Surveying, 1990
Distinguished Service Award, National Council of Examiners for Engineering and Surveying, 1990
Illinois Award, Illinois Society of Professional Engineers, 1997
Loyalty Award, University of Illinois Alumni Association, 1997
Distinguished Service Award with Special Commendations, National Council of Examiners for Engineering and Surveying, 1999

Brent J. Heuser

The Students Award for Excellence in Undergraduate Teaching, 2005

Barclay G. Jones

Fellow, American Nuclear Society
Fellow, Athlone
Honorary Member, Alpha Nu Sigma
Power Engineering Educator Award, Edison Electric Institute, 1991
Outstanding Professor Award, Nuclear Engineering Department, 1998

George H. Miley

Fellow, American Nuclear Society

Fellow, American Physical Society
Fellow, Institute of Electrical and Electronics Engineers (IEEE)
Exceptional Service Award, American Nuclear Society, 1980
Fellow, J. S. Guggenheim Foundation, 1985
Fellow, United Kingdom Research, 1987
Halliburton Engineering Education Leadership Award, University of Illinois College of Engineering, 1990
Distinguished Faculty Member, Alpha Nu Sigma, 1991
Outstanding Achievement Award in Fusion Energy, American Nuclear Society, 1992
Senior Fellow, Japan Society for the Promotion of Science, 1994
NATO Senior Fellow, Eastern European Outreach, 1994
Edward Teller Medal, American Nuclear Society, 1995
Outstanding Scientist Award, *Journal of New Energy*, 1996
Fusion Technology Award, IEEE, 2003
Science and Technology Award, American Nuclear Society, 2004
Associate Fellow, American Institute of Aeronautics and Astronautics, 2005

Magdi Ragheb

Who's Who in the World, 1988

David N. Ruzic

Presidential Young Investigator Award, National Science Foundation, 1985
Andersen Consulting Award for Excellence in Advising, University of Illinois College of Engineering, 1990, 1991, 1992, 1993, 1994
Xerox Award for Faculty Research, University of Illinois College of Engineering, 1990
Everitt Award for Teaching Excellence, University of Illinois College of Engineering, 1992
Stanley H. Pierce Award, University of Illinois College of Engineering, 1992
Oakley Kunde Award for Excellence in Undergraduate Instruction, University of Illinois, 1993
College of Engineering Teaching Excellence Award, 1996
Harriet and Charles Luckman Undergraduate Distinguished Teaching Award, University of Illinois, 1996
Honorary Knight of St. Pat, University of Illinois College of Engineering, 1996
The Broadfick-Allen Award for Excellence in Honors Teaching, University of Illinois, 1997
Graduate College Award for Outstanding Mentoring of Graduate Students Finalist, University of Illinois, 1999

Student Award for Excellence in Undergraduate Teaching,
University of Illinois, 2003

Campus Award for Excellence in Guiding Undergraduate
Research (Honorable Mention), University of Illinois,
2004

Engineering Council Award for Excellence, 2004

Fellow, American Nuclear Society, 2004

Clifford E. Singer

Postdoctoral Fellowship, National Science Foundation

Alexander von Humboldt Fellow, Federal Republic of
Germany

James F. Stubbins

Eminent Engineer, Tau Beta Pi

Alpha Sigma Mu, Metallurgical Engineering Honor
Society

Alpha Nu Sigma, Nuclear Engineering Honor Society

Listed in *Who's Who in Technology Today*

Listed in *American Men and Women of Science*

Rizwan Uddin

Mark Mills Award for Best Ph.D. Dissertation, American
Nuclear Society, 1987

Allan Talbott Gwathmey Memorial Award, University of
Virginia, 1988

ANS Students Award for Excellence in Undergraduate
Teaching, University of Illinois Department of Nuclear,
Plasma and Radiological Engineering, 1998-1999

Young Members Engineering Achievement Award,
American Nuclear Society, 1999

American Nuclear Society Students Award for Excellence
in Undergraduate Teaching, University of Illinois,
Department of Nuclear, Plasma and Radiological
Engineering, 2000, 2001

Campus Award for Excellence in Innovation in
Undergraduate Instruction (Honorable Mention),
University of Illinois, 2004

The Students Award for Excellence in Undergraduate
Teaching, 2005