Laboratory Name: Pacific Northwest National Laboratory
B&R Code: KC020101

FWP and possible subtask under FWP:
Chemistry and Physics of Ceramic Surfaces

FWP Number: 10122

Program Scope:
Experimental activities are integrated with electronic structure calculations that aim to understand surface relaxation phenomena, elucidate the polarity of surface adsorption sites, and simulate molecular conformation and chemical reactivity resulting when a molecule or atom binds to a surface. Research probes the mechanistic and dynamic response of pristine and defected surfaces with carefully designed experiments driven by modeling studies.

Major Program Achievements (over duration of support):
Designed and built a fully instrumented oxide plasma-assisted molecular beam epitaxy chamber for oxide film deposition studies. Showed how certain surface defects promote hydrogen bonding interactions upon absorption of small molecules. Constructed a molecular beam dosing chamber and demonstrated growth of highly porous ice and oxide layers. Deposited and characterized magnetic oxide materials. Developed a high-temperature spintronics thin film with vastly superior magnetic properties than existing materials. 47 journal publications since 2000.

Program Impact:
Published the definitive treatise on the interaction of water with solid surfaces (entire volume of *Surface Science*). Demonstrated how structural and electronic defects influence reactivity at interfaces. Research impacts the effective technological use of oxides as advanced spintronic materials, sorbents for environmental species, as media for interfacial conversion of bound molecules (destruction of environmental contaminants or catalytically-directed product formation), as chemically durable waste forms, as colloidal species in ceramic processing applications, and for a broad range of other industrial applications including sensor and separation membrane development.

Interactions:
Universities: Rod Bartlett (U. Florida); H. Onishi (Kanagawa Acad. Sci./Tech, Sakado, Japan); P.X. Skiba (Austin Peay); A.N. Shultz (Fort Lewis State Univ.); U. Diebold (Tulane Univ.); V. Henrich (Yale); K. Rabe (Rutgers Univ.); C.T. Campbell (UW); E. Altman (Yale); M. Alam (New Mexico Tech.); L. Brillson (Ohio State Univ.);
M. Castro (Univ. Puerto Rico); A. Nilsson (SSRL, Upssala Univ.); C. Fadley, (UC Davis and LBNL); R. Smith (Montana State Univ); M. Gajdardziska-Josifovska, (UW Milw.); C. Hirschmugl, (UW-Milw.); G Brown, Jr. (Stanford Univ. and SSRL). *National Labs*: D.R. Jennison, (SNL); S.H. Overbury, (ORNL); C.L. Perkins (NREL). *Industry*: R. Farrow, IBM Almaden

Recognitions, Honors and Awards (at least partly attributable to support under this FWP or subtask):
Election as Society Fellow: BD Kay (AVS-2000); BD Kay (APS-2000)
University: Adjunct Professor (lqw, bdk, gje); WSU Board of Visitors (gje); WTC Advisory Board (gje)
Technical Meeting Activities: Co-Chair (Conference on Laser-Induced Damage in Optical Materials, 2000, 2001, 2002); General/Program Chair (International Conference on Metallurgical Coatings and Thin Films, 2001, 2002); Symposium Chair: International Vacuum Congress (2001)(gje); Gordon Conf Chair: Surface Dynamics (bdk);
Chair ACS Symposium on Water (bdk); Journal Editor: Appl. Surf. Sci., JVST (sac); Prog. Surf. Sci (bdk); *Technical Society Office*: AVS Board of Directors; AVS Long Range Planning Committee; IUVSTA-Elected Vacuum Metallurgy Division Chair (gje), AVS Surf. Sci. Div. Executive Board (bdk);
(24 invited presentations since FY 2000).

Personnel Commitments for FY2002 to Nearest +/- 10%:
S.A. Chambers (25%); Z. Dohnalek (20%); G.J. Exarhos (10%); K.F. Ferris (20%); M.A. Henderson (25%);
B.D. Kay (20%); L-Q. Wang (25%). Students listed above derived support through this project.

Authorized Budget (BA) for FY00, FY01, FY02:
FY00 BA $ 457K **FY01 BA** $ 414K **FY02 BA** $ 406K

Laboratory Name: Pacific Northwest National Laboratory
B&R Code: KC020102

FWP: Irradiation-Assisted Stress Corrosion Cracking

FWP Number: 12183

Program Scope: The aim of this research is to develop fundamental understanding of radiation damage and corrosion mechanisms controlling intergranular failure of materials exposed to nuclear environments. High-resolution characterization and rate-theory modeling are used to establish relationships among point defects, solutes, microstructure/chemistry, and corrosion reactions. Radiation damage mechanisms affecting grain boundaries are investigated on charged particle and neutron-irradiated materials. Near-atomistic measurements at grain interfaces reveal critical atomic properties that are the basis for materials performance predictions in nuclear energy systems. Current research is focused on complex, multi-component alloys irradiated at intermediate temperatures as well as dose rates where transient behavior influences defect structure evolution and mechanical response. The scientific program goals, and neutron-irradiation activities in particular, are leveraged by collaborations with other DOE-sponsored research and industry projects investigating life-limiting degradation mechanisms in nuclear systems.

Major Program Achievements (over duration of support): Established fundamental understanding of radiation-induced grain boundary segregation in complex alloys through integration of charged particle and neutron experiments. Quantified atomistics of solute-defect interactions derived from rate-theory modeling and high-resolution microscopy/spectroscopy. Elucidated nanometer-scale matrix and grain boundary defect structure evolution during incubation stages of cluster formation. Defined mechanistic linkage between radiation microstructure/chemistry evolution and irradiation-assisted stress corrosion cracking. Created new technique to enable environment-induced crack tips to be interrogated at near-atomic resolution for the first time. Unexpected crack advance mechanisms have been established for structural materials in reactor water environments.

Program Impact: Research has established the basis for current understanding of grain boundary degradation in reactor water environments focused on radiation-induced structure and chemistry changes. This underpinning science is being used as a foundation for control and management of cracking in current nuclear power systems as well as the design of new resistant alloys for advanced reactors.

Interactions: *Internal*—Environmental & Molecular Science Laboratory, Radiochemical Processing Laboratory.
External—University of Michigan (radiation damage mechanisms, proton irradiations); General Electric Global Research (corrosion and stress corrosion mechanisms in high-temperature water); Framatome ANP (grain boundary oxidation mechanisms); University of Minnesota (high-temperature electrochemistry, phase stability and corrosion); Argonne National Laboratory (radiation damage mechanisms); EPRI (neutron irradiations and degraded materials).

Recognitions, Honors and Awards (at least in some part attributable to support under this program):
S. M. Bruemmer – 2000 Fellow of ASM International; Distinguished Service Award (2002) and Secretary/Treasurer (1994-2000) TMS Structural Materials Division; Chairman TMS/ASM Corrosion & Environmental Effects Committee (1994); General/Tech. Chairman (1995-1999), Org. Committee (1990-present) Int. Conf. Environmental Degradation of Materials in Nuclear Power Systems; Org. Committee and Leader Mechanisms Task (1991-), Int. Cooperative Group on Environment-Assisted Cracking; Technical Interpretation Committee Cooperative IASCC Research Group (1994-); Org. Committee Intergranular and Interphase Boundaries in Materials (1998-present); Co-Org. BES/EPRI Research Assistance Task Force on Radiation Materials Science (1998) and NE/BES Workshop on High-Temperature Reactor Materials (2002); Editorial Board for *Metallurgical & Materials Transactions* (2001-).
E. P. Simonen – Chairman for the TMS/ASM Nuclear Materials Committee (1990); ASM Materials Division Council (1992-1993); General Chairman (1993), Technical Chairman (1991), Organizing Committee (1984-present) for Int. Conf. on Environmental Degradation of Materials in Nuclear Power

Systems – Water Reactors; Co-organizer for BES/EPRI Research Assistance Task Force on Radiation Materials Science (1998).

Personnel Commitments for FY2002 to Nearest +/- 10%:
S. M. Bruemmer (30%), E. P. Simonen (50%), D. J. Edwards (25%), L. E. Thomas (25%)

Authorized Budget (BA) for FY00, FY01, FY2002:
FY00 BA $470K **FY01 BA $**424K **FY02 BA $**419K

Laboratory Name: PNNL
B&R Code: KC020102

FWP and possible subtask under FWP:
Interfacial Dynamics During Heterogeneous Deformation

FWP Number: 20009

Program Scope:
Basic mechanisms controlling interfacial deformation of metallic materials are studied and modeled. Emphasis is placed on characterizing, controlling, and simulating dynamic events occurring at grain boundaries, particle-matrix interfaces, and multi-grain junctions during deformation, recrystallization, and recovery. *In situ* microscopy techniques are utilized and atomistic modeling is performed to simulate boundary sliding and junction accommodation. A primary goal of the proposed research is to establish the fundamental science for grain boundary sliding, especially the role of grain junctions.

Major Program Achievements (over duration of support):
Atomistic Modeling of Interfacial Deformation: The effect of the gamma surface on (111) slip has been determined for asymmetric tilt boundaries in Al. There is a symmetry-breaking effect between adjacent (111)-planes, and a [101](111) glide dislocation may be easily incorporated into the boundary on one such plane and blocked on another. The core fields of edge and screw dislocations in Al were determined using EAM methods and fit to a pair of force dipoles characteristic of a dilatant center.
Dynamic Continuous Recrystallization. The microstructural evolution that occurred between strain states of a cold-rolled Al-Mg-Sc alloy was directly observed during *in situ* deformation experiments at 460˚C in the transmission electron microscope. The experiments showed the migration, coalescence, disintegration, and annihilation of dislocation subboundaries in real time. Some of the mechanisms that occur during continuous dynamic recrystallization were documented for the first time.
Fundamentals of Grain Boundary Sliding and Grain Junction Accommodation. Two theoretical papers were prepared this year based on a new CSL approach to grain junctions.

Program impact:
This project has developed numerous new theoretical tools and understanding of grain boundary structure, sliding, and accommodation.

Interactions:
Internal–TEM characterization facilities, Alloy Development Group, Northwest Alliance for Transportation Technologies (NATT) Programs, Computational Materials Science subgroup.
External–CMSN Project, CSP Project, UIUC (Ian Robertson), Brown University (C.L. Briant), SNL and LANL collaborations

Recognitions, Honors and Awards (at least partly attributable to support under this FWP or subtask):
C. H. Henager, Jr. – CMSN Organizing Committee, Invited Presentation at Workshop on Microstructural Effect on the Mechanics of Materials, LANL, 2002.
R. J. Kurtz – Invited presentation at the Second IEA Fusion Materials Workshop on Modeling and Experimental Validation, Les Diablerets, Switzerland, September 30 - October 4, 2002
J. S. Vetrano – Invited presentation at Plasticity 2000, Whistler, B.C., Canada, July 2000, keynote speaker at Thermec 2000, Las Vegas, NV, Dec. 2000.

Personnel Commitments for FY2002 to Nearest +/- 10%:
C.H. Henager, Jr. (50%); J.S. Vetrano (40%); R.J. Kurtz (20%); R.G. Hoagland (40%)

Authorized Budget (BA) for FY00, FY01, FY02:
FY00 BA $ 449K **FY01 BA $** 545K **FY02 BA $** 402K

Laboratory Name: PNNL
B&R Code: KC020102

FWP and possible subtask under FWP:
Fundamental Studies of Stress Corrosion and Corrosion Fatigue Mechanisms

FWP Number: 10757

Program Scope: Develop understanding of the fundamental processes controlling crack tip processes during stress corrosion cracking. Phenomena studied at length scales from nanoscale chemistry at the crack tip to the mesoscale of crack tip deformation and bridging effects. Specific phenomena studied includes impurity segregation, crack-particle interactions, and crack bridging fibers in SiC/SiC composites.

Major Program Achievements (over duration of support): 1) Role of Mg and Cu grain boundary segregation in Al-Mg alloys; 2) demonstrated and modeled the role of anodically active particles in Al-Mg alloys; 3) H permeation rate in Al alloys under electrochemical control; 4) determined the effect of loading mode on crack growth processes; 5) developed a dynamic crack growth model for fiber-bridged cracks in SiC/SiC; and 6) developed a crack growth mechanism map for SiC/SiC based on the PNNL dynamic crack growth model and high-temperature corrosion, creep, and crack growth rate data.

Program impact: Provided significant insight into crack tip processes and the role of Mg and Cu segregation in Al-Mg alloys that are being considered for lightweight automotive applications. Demonstrated that mixed mode loading results in lower toughness than Mode I loading and that H further reduces the toughness under mixed mode loading. Demonstrated that mixed mode loading does not affect stress corrosion crack growth rates in stainless steels. These results have serious implications for all structural materials since standardized testing is done with only Mode I loading. Identified mechanisms of time-dependent crack growth in SiC/SiC composites, and developed a model that matches the experimental data and mechanism maps for effective communication of this information.

Interactions:
Washington State University, (R.G. Hoagland)
Oak Ridge National Laboratory (H.T. Lin)
NASA Glenn Research Center (J. Eldridge)
University of Central Florida (L. Giannuzi)

Recognitions, Honors and Awards (at least partly attributable to support under this FWP or subtask):
D.R. Baer elected Fellow of the American Vacuum Society, 2001
D.R. Baer, PNNL Fitzner-Eberhart Award, 2001
R.H. Jones, chosen to be member of the DOE Peer Review Panel on Waste Package Materials Performance, April 2001 to March 2002.

Personnel Commitments for FY2002 to Nearest +/- 10%:
R.H. Jones, Program Manager, 35%
D.R. Baer, 25%
C.H. Henager, Jr. 30%
J.S. Vetrano, 30%
C.F. Windisch, Jr., 30%

Authorized Budget (BA) for FY00, FY01, FY02:
FY00 BA $ 473K **FY01 BA $** 501K **FY02 BA $** 424K

Laboratory Name: Pacific Northwest National Laboratory
B&R Code: KC-02-01-02-0

FWP and possible subtask under FWP:
Defects and Defect Processes in Ceramics

FWP Number:
18048

Program Scope:
Experimental, ab initio and computer simulation techniques are employed in integrated studies of defect formation, defect migration, defect-defect interactions, and the kinetics of defect-controlled processes in ceramics. Ion channeling, electron microscopy, laser spectroscopies, and X-ray absorption spectroscopies are used to characterize defect properties, kinetics of phase transformations, and nanostructures evolution. Density functional theory and molecular dynamics methods are used to study defect formation, defect migration and damage accumulation.

Major Program Achievements (over duration of support):
Discovered radiation-resistant pyrochlore. Determined defect formation, production, migration, and accumulation processes in SiC. New interatomic potential for SiC. Contributed to understanding radiation damage processes in GaN, $SrTiO_3$, and $A_2B_2O_7$ pyrochlores. New model for irradiation-induced amorphization and disorder accumulation. Determined threshold displacement energies in $ZrSiO_4$ and MgO. 45 journal publications since 2000.

Program impact:
Provided insights on ion-solid interactions and damage accumulation. New SiC potential used worldwide. Provided predictive model for radiation effects applicable to long-term storage of actinide containing waste.

Interactions:
Ab initio calculations and MD simulations – LR Corrales, E.J. Bylaska (PNNL); R. Devanathan (India Institute of Technology – Madras, India); C. Meis, A. Chartier (CEA-Saclay, France); Matthias Posselt (Research Center Rossendorf, Germany); H. Jónsson (University of Washington); L.W. Hobbs (MIT)
Experimental Studies – R.C Ewing and L.M. Wang (University of Michigan); Y. Zhang (Uppsala University, Sweden); A. Hallén (Royal Institute of Technology, Sweden); L.A. Boatner (ORNL); B.D. Begg (Australian Nuclear Science & Technology Organization); E. Alves (Instituto Tecnológico e Nuclear, Portugal)

Recognitions, Honors and Awards (at least partly attributable to support under this FWP or subtask):
W. J. Weber, Organized and chaired Workshop on *Theory and Computer Simulations of Radiation Effects in Ceramics*, Richland, WA, August 1-2, 2002.
W. J. Weber and R. C. Ewing (University of Michigan), Materials Research Society Best Paper Award for Presentation on "Radiation Effects in Crystalline Oxide Host Phases for the Immobilization of Actinides" at the MRS Symposium on *Scientific Basis for Nuclear Waste Management XXV* (2002).
W. J. Weber, Principal Editor and Editorial Board for *Journal of Materials Research* (2002 – present).
W. J. Weber and R. C. Ewing (University of Michigan), Office of Science - Decades of Discovery (top 101 innovations during past 25 years) for research "Preventing Radioactive Contamination" (2001).
W. J. Weber, Guest Co-Editor, Journal of Nuclear Materials, Vol. 289 [1-2] (2001).
W. J. Weber, Elected Fellow of The American Ceramic Society (2000).
W. J. Weber and R. C. Ewing (University of Michigan), 1st Place Winner DOE/BES 2000 Scientific Bullet Award.
W. J. Weber, Co-Organizer, American Ceramic Society Symposium on *Fabrication and Properties of Ceramics for Fusion Energy and Other High Radiation Environments*, St. Louis MO, April 30 - May 3, 2000.
W. J. Weber, International Committee for Radiation Effects in Insulators (1997 - present).

W. J. Weber – 13 invited talks; W. Jiang – 2 invited talks; F. Gao – 6 invited talks (FY00 – FY02)

Personnel Commitments for FY2002 to Nearest +/- 10%:
W.J. Weber (30%), W. Jiang (90%), F. Gao (90%), 2 Visiting Faculty (30% total), 2 Students (25% total)

Authorized Budget (BA) for FY00, FY01, FY02:
FY00 BA $650k **FY01 BA $**551k **FY02 BA $**579k

Laboratory Name: Pacific Northwest National Laboratory
B&R Code: KC020105

FWP and possible subtask under FWP:
Molecularly Organized Nanostructural Materials

FWP Number:
12152

Program Scope:
Research probes novel spontaneous formation processes of nanostructural materials involving molecular-level mixing or nanoscale organization in ceramics, polymers, composites, and blends. The aim is to understand the role of molecular directing agents (surfactants) and their specific interaction with ceramic, liquid or polymer phases at the growing interface during the evolution of ordered nanostructures. Knowledge is used to guide the development of highly functional nanostructural materials with targeted chemical and physical properties including molecular recognition capability, tailored transport properties, or enhanced catalytic behavior. This project addresses basic issues regarding directed structural evolution and the effects of molecular confinement on reactivity and diffusion.

Major Program Achievements (over duration of support):
Surfactant-driven replication of biological structures in ceramic phases spanning length scales from nanometers to millimeters; hybrid nanogels for thermosensitive release of organic molecules; core-shell approach to synthesis of ceramic/polymer materials with controlled nanoporosity; pioneered application of ^{129}Xe NMR spectroscopy for characterization of asperities in materials having interconnected nanoporosity; modeling molecule/surface interactions to understand directed growth and surface mediated conformation; 41 journal publications since 2000.

Program impact:
Molecular understanding of controlled drug release phenomena in nanocomposites driven by second-order phase transformations; acknowledged among the leaders in using magnetic resonance methods to probe structural nuances in nanocomposites; developed chemically-functionalized nanocomposite materials for contaminant sequestration;

Interactions:
Students: Z. Cao (Clemson Univ); Joan Doran (Brown Univ); Candice Willmon (Lewis & Clark College); Jody Rustmann (Colorado College); Anna Ostergaard (Kennewick HS, Col. Basin College); Javier Rameriz (ASU); Anders Wieborg (Gonzaga University); Libby Heeb (Whitman College, UW); Jennifer Cha (U. Cal. Santa Barbara);
Barbara Hoffer (WSU at TriCities).
Faculty: Alex Li (WSU); Burt I. Lee (Clemson Univ); Mira Josowicz (Georgia Tech); Sally O'Connor (Xavier Univ); Igor Moudrakovski (NRC); Raj Bordia (UW)
National Labs: Hau Wang (ANL); Eric Peterson (INEEL); Bruce Bunker (SNL/A); Jun Liu (SNL/A)

Industry: Chet Siew (ADA); Arthur Yang (ITC); John Castle (Nuflo Ind.); Tom Bronkema (Paradyme, Inc.)

Recognitions, Honors and Awards (at least partly attributable to support under this FWP or subtask):
Chunky Bullet Winner: "Nanoporous Materials as Powerful Scavengers for Environmental Pollutants" (gje, jl)
DOE/BES/CSP Project Lead: "Smart Materials Based on Electroactive Polymers" (gje)
University: Adjunct Professor (lqw, wds, gje); WSU Board of Visitors (gje); WTC Advisory Board (gje)
Technical Meeting Activity: Co-Chair (Conference on Laser-Induced Damage in Optical Materials, 2000, 2001, 2002); General/Program Chair (International Conference on Metallurgical Coatings and Thin Films, 2001, 2002); Symposium Chair: International Vacuum Congress (2001) (gje)

Technical Society Office: AVS-Board of Directors; AVS-Long Range Planning Committee; IUVSTA-Elected Vacuum Metallurgy Division Chair (gje). (In addition, 11 invited presentations since FY 2000)

Personnel Commitments for FY2002 to Nearest +/- 10%:
G.J. Exarhos (10%); K.F. Ferris (10%); W.D. Samuels (20%); Y. Shin (30%); Li-Qiong Wang (40%); 2 Visiting Faculty (30% total); 1 post doc (JeongHo Chang). Students listed above derived support through this project.

Authorized Budget (BA) for FY00, FY01, FY02:
FY00 BA $ 300K **FY01 BA** $ 463K **FY02 BA** $ 454K

Laboratory Name: PNNL
B&R Code: KC020301

FWP and possible subtask under FWP:
PNC-CAT Beamlines

FWP Number: 28387

Program Scope:
To support the management and operation of two state-of-the-art beamlines at the Advanced Photon Source designed to address important problems in environmental and basic science. To accomplish this goal, advanced experimental techniques for micro-focusing, imaging, and time-resolved studies have been developed. The PNC-CAT will also serve as a catalyst to involve other government, educational, and industrial organizations in the environmental mission of PNNL.

Major Program Achievements (over duration of support):
The two PNC-CAT beamlines have become operational and are providing beamtime to general users as well as PNC-CAT members. Facilities include an x-ray microprobe with one-micron resolution and advanced detectors, state-of-the-art surface diffraction and XAFS facilities, and a femtosecond laser for time-resolved studies. Over 50 publications have resulted from PNC-CAT beamtime.

Program impact:
The PNC-CAT is providing advanced third-generation synchrotron radiation facilities for research in environmental and materials science.

Interactions:
Internal: A number of groups at PNNL have used the beamlines.
External: Univ. of Washington and Simon Fraser Univ. (CAT members), Idaho National Engineering Lab, Washington State Univ., Univ. of Western Ontario, Univ. of Alberta, Canadian Light Source, Univ. of Oklahoma, SUNY Stony Brook, Univ. of Connecticut.

Recognitions, Honors and Awards (at least partly attributable to support under this FWP or subtask):
Co-chair and proceedings editor: Tenth Int. Conference on XAFS (1998); Chairman Int. XAFS Soc. Committee on Standards and Criteria (2000-present); Steering Committee APS users organization (1998-2001).
Invited talk: *X-ray microprobe studies of Cs and Cr adsorption in Hanford sediments,* 2001 APS Users Meeting, Argonne, IL.

Personnel Commitments for FY2002 to Nearest +/- 10%:
S. M. Heald (40%)

Authorized Budget (BA) for FY00, FY01, FY02:
FY00 BA $ 96K **FY01 BA $** 110K **FY02 BA $** 102K