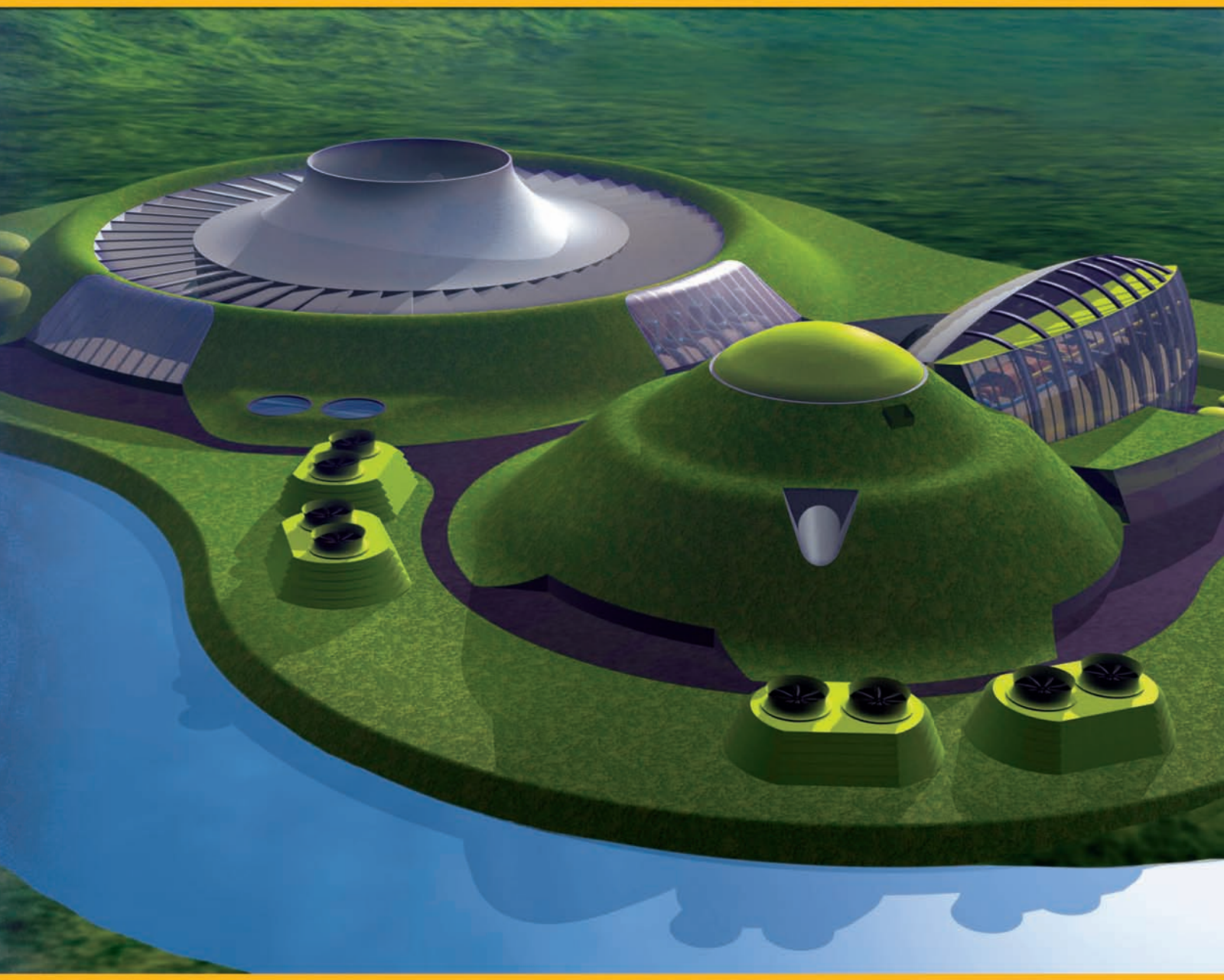
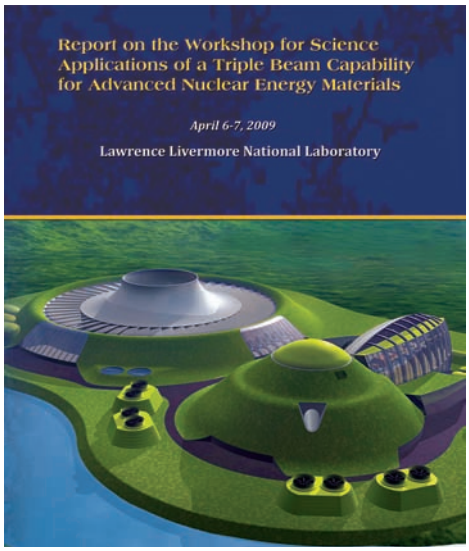
Report on the Workshop for Science Applications of a Triple Beam Capability for Advanced Nuclear Energy Materials

April 6–7, 2009

Lawrence Livermore National Laboratory





About the Cover

Artist's rendering as an idea of how nuclear power plants should be designed in the modern era. (Artist: Aleš Buršic) Cover Image, "Materials Challenges for Advanced Nuclear Energy Systems." MRS Bulletin Vol. 34, No. 1 (2009). Reproduced by permission of the MRS Bulletin.

Workshop on Science Applications of a Triple Beam Capability for Advanced Nuclear Energy Materials

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1. Executive Summary

On April 6–7, 2009, members of the U.S. scientific community interested in irradiation effects on materials gathered at a workshop held at Lawrence Livermore National Laboratory. Their purpose was to discuss the need for a U.S. triple ion-beam irradiation capability to advance the science for nuclear energy materials. The motivation for developing such a capability lies in the complex, highly nonequilibrated situations that are observed in the range of high-radiation environments associated with advanced nuclear energy systems (ANES), including fission, fusion, and nuclear waste environments. In these environments, materials not only undergo radiation damage but also experience changes in their chemistry as the concentration of hydrogen, helium, and other transmutations increases.

Ion beams are of great use in experimentally simulating complex, high-radiation environments. Among their many advantages is that they greatly accelerate the damage process compared to available neutron sources or the self-radiation damage in nuclear waste materials, while leaving samples in a nonradioactive state. These abilities enable scientists to effectively use ion beams to understand the fundamental radiation effects mechanisms of complex ANES environments. However, there is evidence that *sequentially* irradiating materials with heavy ions (to create radiation damage), protons (to inject hydrogen), and He^- does not produce conditions that are relevant to ANESs, where damage and the build-up of H and He occur *simultaneously.* The occurrence of possible synergistic effects has prompted scientists in France, Japan, and the Ukraine (see Figure 1, Figure 2, and Figure 3) to develop the capability to simultaneously irradiate materials with two or three ion beams: heavy ions, and one or two other energetic beams representing the transmutants.

There were four major outcomes of the workshop:

1. Participants agreed that a triple ion-beam facility would play an important role in training the scientific leaders of the future. Irradiation damage experiments at neutron sources or using short-lived radionuclides in waste forms can last for a long time, having timeframes that are inconsistent with that of a doctoral graduate student's matriculation. Additionally, sample space in neutron sources is quite precious and can be difficult to obtain. Irradiations can take months or years to reach desired doses. Finally, samples are radioactive when removed from the neutron source and may need to cool for months before experiments can be carried out. In contrast, ion irradiation has the advantage of high displacement and simulated "transmutation" rates with little to no activation. Experiments can be carried out very efficiently and samples can be characterized in situ or immediately after irradiation.

2. Participants clearly stated the important role that ion beams play in advancing our fundamental knowledge of irradiation effects. Ion beams are invaluable because they provide a research platform for investigating the fundamental mechanism underpinning radiation effects in ANESs. They provide control of variables that will allow investigation of unit mechanisms. Therefore, part of this report examines the basic research that would be catalyzed by the existence of a U.S. triple ion-beam facility.

3. The community is keenly interested in experiments where mechanisms can be probed in real time, in situ. This included a strong endorsement of the capability for in-situ, multiple-ion-beam irradiation in an electron microscope, as well as the usual ion-beam techniques (channeling, PIXE, ERDA, NRA, RBS, etc.).

4. Attendees acknowledged the central role that theory, simulation, and modeling will play in understanding data generated at a triple ion-beam facility. Damage effects due to ion beams can be realized three orders of magnitude faster than those occurring in reactors, and eight to ten orders of magnitude faster than in nuclear waste forms, thereby allowing high-dose effects to be studied in realistic timeframes. Experimental comparisons with theoretical predictions as a function of variables such as energy, temperature, and dose rate will provide critical tests of our understanding of the unit mechanisms and our ability to bridge time and length scales using modeling and simulation.

Through a survey of the participants, it was estimated that the user community would initially include about 200 professionals, post-doctoral researchers, and graduate and undergraduate students. About one-half of the users would come from national laboratories and one-third from universities. Twenty-five percent of the users have support from BES. Twenty-five percent of the users have support from NE. Ten percent derive their support from FES. A full three-quarters of the use would be in the discipline area of materials science. In many cases, specimen fabrication would require use of special capabilities at BES national nanocenters. Materials irradiated at a triple ion-beam facility would spawn post-irradiation experiments at many of the BES scientific user facilities, including neutron sources, photon sources, and electron microscopy centers.

The workshop participants indicated near unanimous support for a U.S. triple ion-beam irradiation capability that would be operated as a user facility. The characteristics proposed for such a user facility will be discussed in more detail in the following report.

2. Introduction

2.1. Purpose of the Workshop

Lawrence Livermore National Laboratory hosted a workshop on April 6 and 7, 2009 in Livermore, CA, which focused on the *Science Applications of a Triple Beam Capability for Advanced Nuclear Energy Materials.* Workshop participants are listed in Appendix A and the agenda is provided in Appendix B. The motivation for this workshop was aligned with many of the goals and objectives described in *"Basic Research Needs for Advanced Nuclear Energy Systems"* (ANES) of July 31–August 6, 2006.[1] The ANES report notes: *"Revolutionary research is called for that enables and utilizes an integrated approach of experimental and modeling efforts in designing radiation-resistant materials and predicting the response of materials in extreme environments… New models are needed to treat the complexities of real alloys in extreme conditions. Similarly, new experimental developments in validating models at the appropriate time and length scales and for providing critical data model input are needed."*

In the ANES report's executive summary of workshop Panel I, "Materials Under Extreme Conditions," a compelling argument is made for the synergistic integration of unique experimental platforms with advanced theory, simulation, and modeling: *"The goal of designing radiation-resistant materials for extreme environments will require the development of advanced computational models that are valid over length and time scales that vary from less than nanometers and picoseconds to over millimeters and years... The success of this methodology will require development of new experimental capabilities that can test model predictions and provide input to the models at all relevant length and time scales. At the same time, new models must be developed that can treat the complexities and nonlinearities of complicated alloys in arbitrary irradiation environments."*

What is a triple beam accelerator?

Historically, facilities for studying the effects of ion beam irradiation have housed single-beam, heavy ion or light ion accelerators and target chambers outfitted with diagnostic capabilities. Such facilities have provided great insight into the production and accumulation of radiation damage.
With interest in understanding the damage that might occur in nuclear reactors under fast neutron and high fuel burnup conditions growing, the synergies that may exist among radiation damage and fission products or transmutants become important.

By coupling a heavy ion accelerator that provides ions in the 10–100 MeV range with two lower-energy accelerators for implanting gas ions such as H and He, it may be possible to begin to unravel the complex microstructural and microchemical evolutions that are expected in advanced nuclear energy systems. In cases involving materials that are susceptible to radiolysis, an electron beam may also be used to produce ionization damage.

The energy of the heavy ions is chosen to optimize penetration in bulk-like samples. The light ion energies are chosen so that the ions implant at the desired depths and intersect the displacement damage from the heavy ions.

As noted by Panel IV of the ANES workshop, the scientific challenge in the development of advanced fuels lies in developing the underlying fundamental science base—an area where innovative experiments and experimental platforms can make full use of advances in all aspects of materials theory, simulation, and modeling. An approach that couples theory, simulation, modeling, and experimentation would serve to develop this fundamental science base, which would enable a transition away from lengthy and costly empirical methods. Instead, the focus would be on understanding and predicting the interplay of the nuclear, chemical, and thermomechanical phenomena that determine fuel evolution.

A triple ion-beam facility is one platform that, when coupled with theory, simulation, and modeling, will help address the challenges presented by structural and fuel cladding materials as well as advanced nuclear fuels and subsequent waste forms.

2.2. Further progress requires a triple ion-beam capability

Nuclear power—whether employing fission, fusion, or spallation technology—and nuclear waste disposition both require a fundamental understanding of structural alloys and fertile, fissile, and fission product materials that can survive extreme environments for long periods—from decades to centuries or even millennia, without failure. In addition to exposure to high temperatures and corrosive environments, these materials must withstand high levels of bombardment by neutrons. Neutron irradiation causes atoms to be displaced from their lattice sites and produces vacancies and interstitial atoms, both of which are highly mobile and can contribute to extensive microstructural and microchemical changes in the material. In concert with transmutations resulting from (n,α) and (n,p) nuclear reactions, these changes usually degrade the original mechanical and physical properties of the materials. These changes can also produce substantial instability in material dimensions and volume. Such changes in both properties and dimension often become the life-limiting determinant of materials in advanced nuclear energy systems.

In a neutron irradiation environment, the driving force for microstructural and microchemical processes is the combined effect of atomic displacements with helium and hydrogen production. It is traditional practice (although not necessarily rigorous scientifically) to define the irradiation dose in terms of "displacements per atom," or dpa. An exposure of 20 dpa means that, on the average, each atom in the material has been displaced from a lattice site 20 times. As reactor technology evolves, with increases in nuclear efficiency and closing of the fuel cycle, the maximum dpa of ~1 for first-generation fission reactors is now only a small fraction of the anticipated damage that will be encountered in advanced nuclear energy systems (see Table I). To reach maximum burnup[1], fuel-cladding alloys must endure doses significantly greater than 100 dpa. For most fast reactor applications, 200–250 dpa is required. Table I also gives the He and H concentrations that are expected because of transmutations. These figures emphasize the point that hydrogen concentrations in fast neutron spectra are potentially an important issue.

[1]Burn-up is a measure of the number of fuel atoms that have undergone fission.

	Fission (Gen I)	Fission (Gen IV)	Fusion (DEMO/PROTO)	Spallation (ADS)
Structural alloy T_{max}	<300 °C	300–1000 °C	550–1000 °C	140–600 °C
Max dose for core internal structures	~1 dpa	~30–200 dpa	~150 dpa	50–100 dpa
Max helium concentration	0.1 appm	~3–40 appm	~1500 appm (~10,000 appm for SiC)	~5000 appm/fpy
Max hydrogen concentration			~6750 appm	50,000–100,000 appm/fpy
Neutron Energy E_{max}	<1–2 MeV	<1–3 MeV	<14 MeV	Several hundred MeV

Table I. The dpa fluence or dpa rate encountered in various neutron technologies is shown, along with the helium and hydrogen transmutation. Some modifications to the source reference to this table have been made here in the Spallation ADS column.[2] fpy = full power year. T_{max} = maximum temperatures for structural alloys.

The successful development of radiation-tolerant materials is guided by progress in understanding the basic physics involved in the process of radiation tolerance; an example is the impressive progress achieved in the design of ferritic steels with nano-scale dispersed oxide particles.[4] The composition and morphology of these particles and their role in radiation tolerance remain topics of current research, i.e., the reason for their radiation endurance is unknown (for example, see [4–11]).

Additionally, the importance of the role of multiscale modeling in researching radiation tolerance cannot be overstated.[12] This approach has raised expectations based on the spectacular progress achieved in the last few years. Although we do not yet have the ability to fully model what happens in a real material under irradiation with quantitative predictability, nor can we design right from the computer a radiation resistance material, every day we are closer to achieving these goals. In the years since the pioneering work of R. S. de Groot and others in the 1940s and 1950s, which laid the foundation of the theoretical approach to the thermodynamics of irreversible processes,[13–18] an impressive body of research has been developed that today focuses on the study of the emergence of complexity in open (driven) systems. When these concepts are applied to radiation damage, it is possible to imagine materials in which irradiation continuously deposits energy while intrinsic thermodynamic processes heal the damage in a way leading to stationary states. Such materials were suggested by the pioneering work of G. Martin et al. in the 1990s,[19–21] and were recently suggested by Demkowicz et al.[22] to be the case in CuNb multilayers.

To understand and model the aging caused by atomic displacements, helium and hydrogen production, and transmutations, material scientists and reactor engineers usually irradiate candidate nuclear reactor materials in nuclear reactors. Descriptions

of several such facilities can be found in Table II. Unfortunately, such an approach takes much too long, as there are no neutron sources available in the U.S. to sufficiently accelerate the aging process. Employing a triple ion-beam circumvents this limitation by enabling accelerated aging of materials through multibeam ion irradiations. Multibeam irradiations produce displacements along with requisite helium and hydrogen implantation, thus assuring that synergistic effects are not overlooked in these experimental simulations of neutron damage. While the outcome of these types of experiments is not necessarily equivalent to neutron damage, the experiments have the power to put in evidence physical processes to spark our imaginations and challenge our models.[23] A relevant example of this is the recent triple-beam experiments by Tanaka and coworkers.[3] The authors report the synergistic effects of iron ion-damage along with simultaneous He and H implantation resulting in significantly greater swelling than corresponding dual-beam experiments of iron ions with either He or H implantation. See Figure 1.

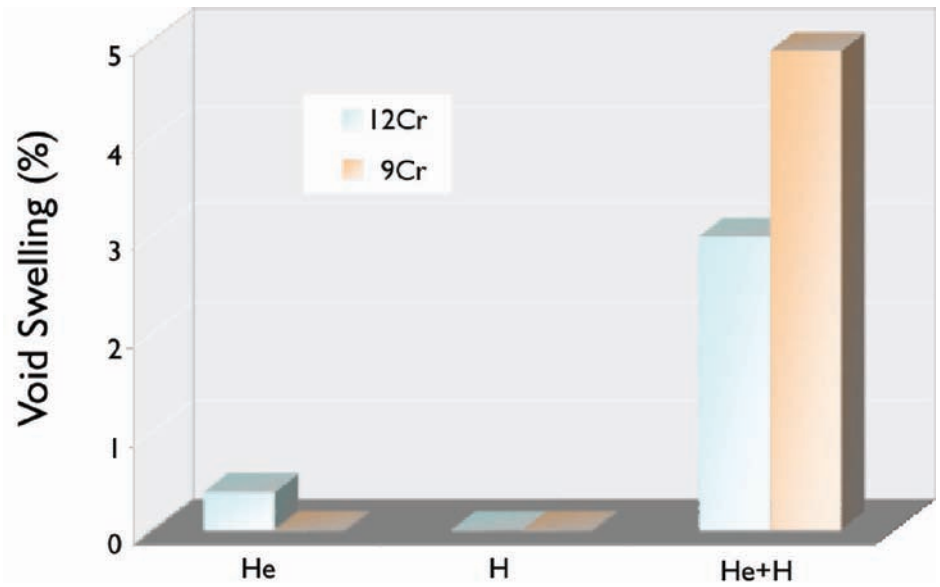

Figure 1. The synergistic effect of He and H was shown clearly in the triple ion (Fe^{3+} + He^{+} + H^{+}) irradiation of an FeCr steel.[3]

Facility	Country	Fast Flux E_n>0.1 MeV ($10^{18}/m^2s$)	Displacement damage in steel (dpa/yr)	Useful vol (cm^3)	Temp Range (°C)	Comments
BR2 Core Reflector	Germany	 1.5–3.0 0.05–1.0	 <3/yr <1/yr	 90 250	 50–1000 50–1000	• ~105 days/yr • Caps ϕ: 50–200 mm • In-situ fatigue rigs
OSIRIS	France	2.5	few/yr	230	50–1000	
HFR Core (C5)	Nether-lands	 2.5	 <7/yr	 1540	 80–1100	• 275 days/yr • In situ experiments
ATR A and H, B, I-positions Flux traps	U.S.	 2.3 0.8 0.03 2.2	 6–10/yr 6–8/yr	 240 1390 5560 5560	 50– >1500	• Caps ϕ: <127 mm • Large irrad. volume • Versatile facility
HFIR Tgt. Pos 37 RB pos 8	U.S.	 11 5.3	 18/yr 5–7/yr	 100 720	 300–1500	• Very high peak flux • Accelerated testing in smaller volumes
JOYO	Japan	5.7	~30/yr		300–700	• Temp. control +4 K • 300 days/yr
BN600	Russia	6.5	20-52	350	375–750+	• Very-high dose rate • Only passive instrumentation
BOR-60	Russia	3.0	~20	358	300–700+	• Only passive instrumentation • High level PIE

Table II. A sampling of currently active reactor facilities worldwide used for materials testing. The first five reactors listed are considered mixed-spectrum reactors, while the last three are fast reactors (*from ref* [2]).

In addition to a triple ion-beam facility, two important variations in the application of multiple ion beams and in the configuration of multiple ion-beam facilities were discussed at the workshop:

1. The integration of multiple ion beams with electron microscopes.

2. The use of multiple ion beams to control the development of nanostructured materials.

2.3. Ion beams for use-inspired basic research

As discussed in Section 2.2, it will be difficult to develop and qualify materials for ANESs using conventional neutron sources because the dose rate is simply too low. It will require one to two decades to reach the required high doses of most advanced nuclear energy systems using existing nuclear test reactors (see Table II). Because material development usually takes several iterations of irradiation, testing, and modification before an optimum material can be qualified for use in a reactor, perhaps three decades will be required. This lengthy time requirement is one of the most vexing issues standing in the way of nuclear energy development for the future.

An alternate approach for investigating radiation performance at high dpa is to use charged particle irradiation at greatly accelerated dpa rates (~10^3 times faster than neutrons from available sources) to simulate neutron damage. This approach has been used successfully to study many aspects of void swelling, phase-stability, and irradiation creep. The advantages of this approach are significant:

1. The damage rate is higher than for neutrons from available neutron sources.

2. The control of experimental parameters (temperature, flux, energy, and environment) is far better than can be achieved in-reactor.

3. Irradiated specimens are generally not radioactive, unlike reactor specimens that may be highly radioactive and require examination in hot cells.

To illustrate the potential capabilities of a triple ion-beam facility, three existing facilities are described as examples. Figure 2 shows the TIARA triple ion-beam facility in Japan. The facility has three accelerators arranged to allow one, two, or three beams to enter either of two chambers, one for intermediate-temperature experiments and one for high-temperature experiments. The system incorporates beam sweepers, degrader foils, and dosimetry as well as in-situ diagnostics such as Rutherford Backscattering (RBS) and infrared thermometry. Figure 3 illustrates the multipurpose layout planned for the Saclay JANNuS triple ion-beam facility.[24] The use of an electron cyclotron resonance (ECR) source will allow for high current and high energies from multiply charged ions (e.g., $Fe^{>8+}$). This facility will use a target chamber similar to that at TIARA. The facility is expected to be operational early in 2010. Figure 4 shows the triple ion-beam facility at Kharkov University in the Ukraine. This facility is more modest and makes use of compact helium and hydrogen ion sources along with heavy ions from an electrostatic accelerator. A triple ion-beam facility existed previously in the U.S.[25] and was used to carry out a range of experiments.[26] Other dual beam and transmission electron microscope (TEM)–ion-beam facilities are tabulated in Table III.[27] Appendix C provides a more in-depth discussion of international facilities.

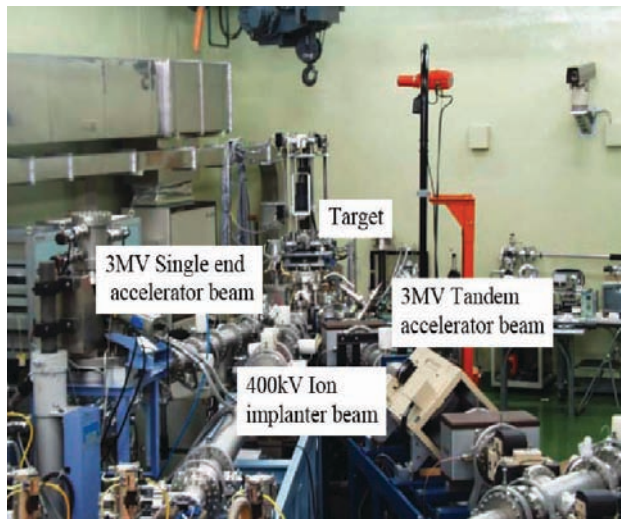

Figure 2. The TIARA (Takasaki Ion Accelerators for Advanced Radiation Applications) triple beam facility. The facility consists of a 3-MV single-ended accelerator, a 3-MV tandem accelerator, and a 0.4-MV ion implanter.

Some aspects of charged particle irradiation produce behavior that is atypical of that produced by neutrons at lower dpa rates. Examples of atypical behavior are: the injected interstitial effect,[28,29] the proximity of specimen surfaces to the damaged volume, beam heating, and phase and microstructural evolution that is sensitive to displacement rate and/or irradiation time. To varying degrees, the influence of these atypical variables can be modeled. When data from accelerated charged particle irradiation is combined with theoretical modeling, especially when using computer simulation on the scale of the microstructure, it would appear that significant understanding of the response to irradiation in both charged particle and neutron environments can be derived, thereby allowing better interpretation and extrapolation of the results to the neutron environment.

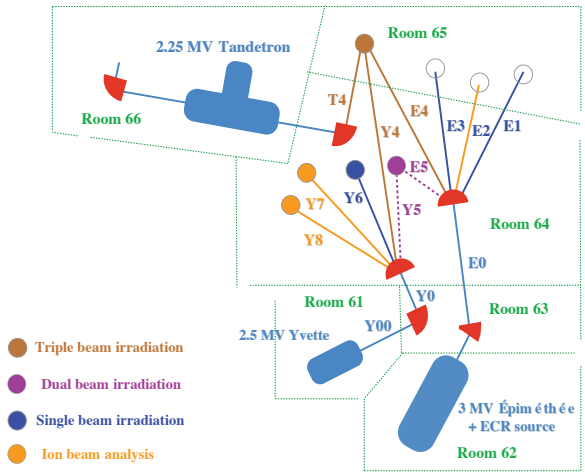

Figure 3. JANNuS CEA-Saclay is a versatile triple ion-beam facility. Ion species and intensities typical of the facility are as follows: maximal intensities delivered to the targets will be at least 3.9×10^{14} pps (particles per second) for protons, 8.8×10^{14} pps $^{4}He^{+}$, 2.2×10^{14} pps $^{4}He^{2+}$, 1.8×10^{12} pps $^{132}Xe^{10+}$, 3.10^{11} pps and 8.2×10^{12} pps $^{40}Ar^{8+}$, $^{56}Fe^{8+}$ 2.6×10^{12} pps or $^{58}Ni^{11}+$ 1.1×10^{12} pps.

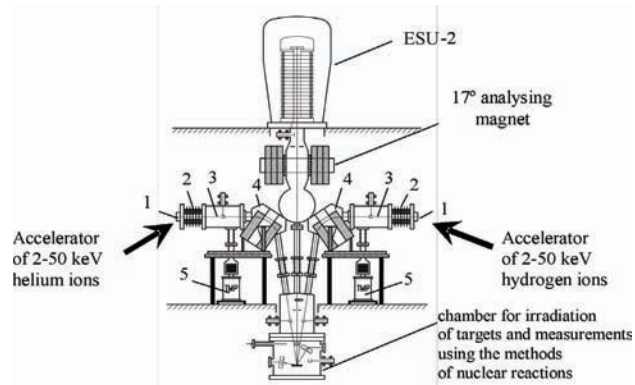

Figure 4. Diagram of measuring complex ESU-2 at the National Science Center Kharkov Institute of Physics and Technology. 1 – ion injector; 2 – accelerating system; 3 – base chamber; 4 – electromagnet; 5 – turbomolecular pump.

Multiple-irradiation facilities available in the world

Laboratory	Facilities	Application field	Reference
a) dual or triple MeV ion beams			
MSD, IGCAR, Kalpakkam, India	1.7 MV Tandetron	Irradiation behavior of nuclear alloys Ion implanter (30–150 keV)	[30]
HIT, Tokyo, Japan	3.75 MV Van de Graaff 1 MV Tandetron	Irradiation behavior of nuclear alloys and ceramics	[31]
DNE, Nagoya University, Japan	2 MV Van de Graaff 200 kV ion implanter	Irradiation behavior of nuclear alloys and ceramics	[32]
FZ, Rossendorf, Germany	3 MV Tandetron 500 kV ion implanter	Synthesis of nanostructured ceramics assisted by irradiation Ion beam modification of materials	[33]
FSU, Iena, Germany	3 MV Tandetron JULIA 400 kV ion implanter ROMEO	Synthesis of nanostructured ceramics assisted by irradiation Irradiation behavior of nuclear alloys	[34]
IAE, Kyoto, Japan	1.7 MV Tandetron 1 MV Van de Graaff 1 MV Singletron	Evolution of microstructure under multi-irradiation	[35]
JAEA, Takasaki, Japan TIARA	3 MV Tandem 3 MV Van de Graaff 400 kV ion implanter	Synthesis of nanostructured ceramics assisted by irradiation Behavior of alloys and ceramics under irradiation	[36]
DMN, Saclay, France JANNuS (ready to operate at the beginning of 2009)	3 MV Pelletron ÉPIMÉTHÉE 2.5 MV Van de Graaff YVETTE 2.25 MV Tandetron	Irradiation behavior of nuclear materials Ion beam modification of materials	[27]
Kharkov Institute of Physics and Technology, Kharkov, Ukraine	2 MV ESU 50 kV proton 50 kV helium	Irradiation behavior of nuclear alloys	[37]
LANL, USA	3 MV Tandem 200 kV ion implanter	Heavy ion irradiation from the tandem Simultaneous He/H implantation from the implanter	[38]
b) mono or dual ion beams (>100 keV) coupled to a TEM			
CARET, Sapporo, Japan	1.3 MV HVTEM 400 kV ion implanter 300 kV ion implanter irradiation	Synthesis of nanostructured materials assisted by irradiation Behavior of nuclear materials under	[39]
Argonne National Laboratory, USA	2 MV Tandem or 650 kV ion implanter 300 kV TEM	Irradiation behavior of nuclear ceramics	[40]
CSNSM, Orsay, France (will operate at the beginning of 2008)	2 MV Tandem Van de Graaff ARAMIS 150 kV ion implanter IRMA 200 kV TEM	Irradiation behavior of nuclear ceramics and semiconductors Ion beam modification of materials	[27]
c) dual keV ion beams coupled to a TEM			
IMR, University of Salford, UK (under construction)	200 kV TEM Ion implanter (5–100 keV, A ≤ 140)	Radiation damage on nuclear reactor materials and semiconductors	[41]
JAERI DMD, Takasaki, Japan	400 kV TEM 400 kV ion implanter 40 kV ion gun	Radiation effects	[42]
JAERI DMSE, Tokai-Mura, Japan	2°—40 kV ion guns 400 kV TEM	Irradiation behavior of nuclear alloys and ceramics	[43]

Table III. A list of the various multi-ion-beam and ion-beam–TEM facilities in the world. (*Most of the content comes from ref* [44].)

3. Scientific Challenges

A summary of discussions among workshop participants, whose inputs underpin this section, can be found in Appendix D. Scientific challenges submitted by participants are described in Appendix E. Correlation and binning of those challenges can be found in Appendix F. Participants in the workshop emphasized that a triple ion-beam capability would be an important tool for basic materials research. Therefore, in Appendix G we have correlated the workshop output with both Basic Energy Sciences Advisory Committee (BESAC) grand challenges[45] and BES basic research needs.[1,46]

3.1. Scientific Challenge 1: Microstructural and synergistic effects of high displacement damage coupled with implantation of transmutation products

Atomic displacements alone, while a convenient scaling factor, do not represent the full nature of the radiation environment for the structural and cladding materials of nuclear energy systems. Indeed, it is well known that there are complex synergies at play in the evolution of the microstructure (and hence the properties of materials) in a nuclear energy system, although the synergies are not understood.[3,47] Therefore, while ion-beam irradiations are well suited to isolate unit mechanisms associated with the complexity of radiation damage accumulation, it is essential that an experimental platform also be able to mimic those synergies that may be critical in developing a comprehensive understanding of the details of the mechanisms active in a particular microstructural evolution.

Despite continuous progress in understanding the basic mechanisms of radiation damage, there is still much to learn before we gain the level of understanding that will allow us to predict the evolution of materials over the time, temperature, and length scales associated with modern-generation nuclear energy systems, both fission and fusion. Recent investigations of radiation damage phenomena have made remarkable progress. (A recent summary of progress and challenges can be found in [48] or [49], which describe the use of ion beams to discover a class of radiation-resistant pyrochlore ceramics suitable for immobilization of actinide waste.) Charged-particle or ion-beam studies that can mimic the complex radiation, temperature, chemical, and mechanical environments of a material in a nuclear energy system can be critical scientific adjuncts to advancing our fundamental understanding of radiation effects in materials, indeed materials under extreme conditions.

One of the most intriguing scientific challenges is the interaction of hydrogen and helium with the evolving defect structure, and with one another, in a solid under continuous radiation. In a reactor, the hydrogen and helium arise from nuclear reactions (n,p) and (n,α). Hydrogen can be produced from the hydrolysis of water in contact with a material. The amount of hydrogen and helium produced by nuclear reactions depends on the nuclear properties of the target material and the energy of the impinging neutron, unless it is a transmutation reaction with thermal flux, such as ^{59}Ni interaction. Generally, the faster the neutron spectrum the more hydrogen and helium are produced. In the past, the hydrogen in thermal reactor stainless steels has not been considered as important. Recently however, Garner et al. have shown that unexpectedly high concentrations of hydrogen are found in stainless steels from thermal fission reactors.[50] It would not be surprising to discover that the mysterious effects associated with synergy could be replicated with well-chosen sequential irradiations. However, the discovery and understanding of such effects is important, and only by having an experimental facility where such experiments can easily be executed will we avoid discovering such effects much later in the R&D process, and with much higher cost consequences.

There is now experimental evidence from triple ion-beam experiments where the synergistic effect of displacement damage, along with helium and hydrogen, enhances one or more of the aspects of microstructural development from irradiation-induced damage.[51,52] We noted earlier the data of Tanaka et al.[3] where high swelling was observed in ferritic model alloys of FeCr under triple ion irradiation. Similar results in V alloys have been reported by Sekimura et al.,[47] where simultaneous irradiation of Ni, He, and H ions enhanced void formation and swelling. Triple ion irradiation has been shown to lead to greatly enhanced swelling of F82H martensitic steel (an 8Cr-2W steel), compared with dual beam irradiations of hydrogen and heavy-ion or helium and heavy-ions.[53] Since hydrogen is very mobile in these steels, the reasons for this hydrogen accumulation are a topic of scientific debate. It appears to be synergistically related to helium retention, but further research is required to understand whether the consequences are important to advanced nuclear energy concepts, both fusion and fission.

Another area of scientific challenge is the role that nanostructures (see Figure 5) play in radiation tolerance. It is believed that for the oxide dispersion strengthened (ODS) steels, the oxide dispersoids of a few nanometers help in the role of helium management. Unfortunately, the details of the mechanism(s) by which this is accomplished remain a mystery and hence an important scientific challenge. What the role of hydrogen would be if introduced simultaneously with displacements and helium, of course, is just as much a mystery calling for fundamental experiments and modeling. Such irradiations of ODS materials, coupled with advanced microscopy characterization with ultra-high resolution instruments, will result in the fundamental science needed to understand, model, and quantitatively predict performance for radiation-tolerant materials in advanced nuclear energy systems.

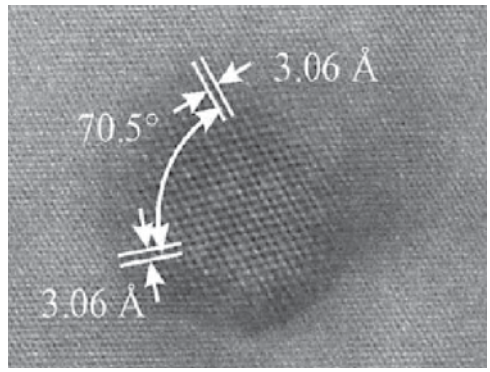

Figure 5: A high-resolution electron microscope image of a nanodispersoid particle in an Fe(Cr) steel.

In order to expose the underlying physics of irradiation in structural materials, one must know the detailed microstructural processes that are active. Performing these irradiation experiments on thin foils in real time within a TEM will permit direct observation of the active mechanism and microstructural rearrangements that occur. The concurrent implantation of heavy ions, H, and He in a TEM will permit a greater understanding of the nucleation and growth mechanisms of defect structures such as gas bubbles found in irradiated structural materials. The detailed understanding provided by these experiments will permit significant furthering of models that predict the lifetime of nuclear fission and fusion reactors. Beyond this significant addition to nuclear reactor models, the fundamental understanding of interactions in irradiated solids can be gained by combining these proposed in-situ TEM irradiation studies with simultaneous annealing and straining experiments. The potential combination of heavy ion, He, and H irradiation with both annealing and straining experiments during direct observation via a TEM would permit the greatest insight into the microstructural rearrangement that occurs in nuclear reactors. In this regard, it is expected that these in-situ measurements will be highly synergistic with the ex-situ experiments, and may even be required to fully understand the evolution of microstructure and mechanical properties observed by the ex-situ measurements.

3.2. Scientific Challenge 2: Evolution of microstructure, physical, and chemical properties in complex actinide fuels and nuclear waste management materials

3.2.1. Advanced fuels

The design and fabrication of advanced materials, coupled with validated modeling, is essential for establishing nuclear energy as a cost-effective and sustainable supply of clean energy. This is particularly the case when it comes to maximizing fuel energy usage, optimizing fuel power density and thermal transport, and reducing nuclear proliferation and waste—all of which are key components to advancing nuclear energy. Future generations of advanced fuel cycles will require that we have a fundamental knowledge of high burnup fuels. Systematic studies of high burnup fuels will provide basic knowledge that will position the U.S. to take a leadership role by leveraging our actinide fabrication and characterization facilities and our world-leading computational capabilities with our best-in-class modeling and simulation.

Many fuel types have been proposed for ANES: oxides, carbides, nitrides, a ceramic and metal inert matrix, and SiC-pyrolytic carbon tri-isotopic fuel pellets. For any of these variants, using multiple ion-beams in well-designed experiments could lead to developing a scientific basis for understanding and modeling the complex evolution of the fuel in nuclear energy systems, where a large fraction of the fissile and fertile atoms undergo fission. Diffusion couples based on binary and ternary compounds can be exposed in irradiation environments at temperature. This will permit key thermodynamic and kinetic parameters to be determined for the first time. Quantitative structural and mechanical characterizations will provide direct input and validation to the modeling at high burnup. Ion-beam irradiation of both the actinide fuel and any inert components or additives, at fission product energies, are key experiments for additional scientific investigation. Experiments will quantify phase transformations and phase stability, microstructural evolution, thermal conductivity, mechanical properties, and the influence of severe radiation environments on fuel performance.

Thermodynamic and kinetic modeling should be used to predict the stability and time evolution of phase transformations and reactions associated with complex materials exposed to a changing chemistry in high burnup fuel. This knowledge will establish the scientific basis for high-throughput search methodologies for optimized nuclear fuel compositions by monitoring microstructural phase evolution in extreme conditions of radiation, temperature, and extended time. This modeling could be interfaced to an experimentally validated first-principles description of defect formation and migration energies in both the alloys and fission product compounds. The challenge is to have a validated model of the evolution of advanced nuclear energy materials under extreme conditions of radiation, temperature, and evolving chemistry—a model that is founded on a science base and that leads to the development of a validated nuclear fuel database and, in turn, to optimized fuel forms for high burnup (e.g., see [54]).

As noted in [1], the science challenge consists of developing a fundamental science base that changes the fuel development paradigm from time-intensive and costly empiricism to science-based fuel development and qualification. To meet this challenge, we must make full use of advances in electronic structure theory, computational thermodynamics, and innovative, science-driven experiments to obtain the required understanding of fuel materials and their evolution during high burnup. The obstacle facing the materials scientist is to develop a fundamental understanding of a complex, multicomponent, multiphase materials system that irradiation is driving far from equilibrium. The materials challenge for advanced nuclear energy fuels is daunting but not impossible. We expect to be able to meet this challenge using multiscale modeling and carefully de-

signed experiments that yield important materials parameters to guide, verify, and validate the models. Probably the most important synergy problem is the concept of incubation, which usually involves a complex set of differential equations arising from the many facets of the radiation, dpa, helium, and hydrogen. The fundamental issue is to understand their time- and concentration-dependent interactions. If the interaction times are short, sequential irradiations will not adequately reveal or mimic the underlying mechanisms. Access to a flexible experimental platform that can mimic the complexity of radiation-induced damage is crucially important.

3.2.2. Waste forms

The science challenges associated with nuclear waste materials are somewhat similar to those of nuclear fuel research. However, there are many more differences than there are similarities. The primary difference is the extraordinary time scale for nuclear waste storage: not decades, as for nuclear fuel lifetimes, but millennia. The principal sources of ionizing radiation are alpha particles, beta decay, and gamma rays; alpha particles and alpha-recoil nuclei are the principal sources of atomic displacements from ballistic damage. Hence, experimental facilities that can accelerate the processes involved and allow observation of the complex evolution of the waste form are very desirable.

Because interfacial phenomena are important in the evolution of nuclear waste forms, experiments that allow in-situ observation under simulated radiation conditions are extremely valuable in advancing the science. An example of such an experimental set-up is the use of a high-voltage electron microscope as both an observational tool and as an irradiation source coupled with one or more ion-beams. Figure 6 shows an example of such an advanced research tool in Japan being operated by a U.S. waste-form researcher. In this work,[55] the unexpected synergy of helium and electron radiation simultaneous with xenon-produced radiation damage was observed, demonstrating the discovery-class research that can only come from such an experimental platform (see Figure 7). There are no equivalent dual ion-beam–TEM facilities available to researchers in the U.S., as shown in Table III.

In addition to experimental facilities, theory simulation and modeling are also vital. Low dose rates represent a grand challenge for predictive modeling. It is essential that we build a fundamental basis that couples electronic and nuclear stopping in order to understand long-term irradiations in waste storage materials.

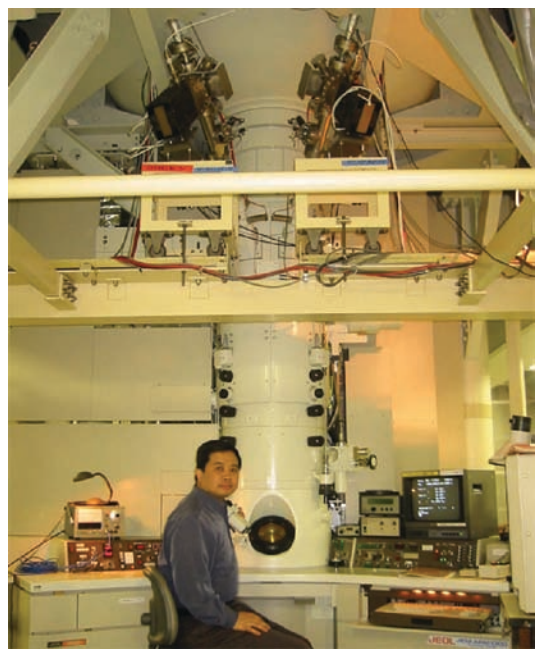

Figure 6. Professor Lumin Wang, University of Michigan, at the console of the multibeam HVEM irradiation facility at Hokkaido University, Sapporo, Japan (two ion beams and an electron beam). No such facility for advancing the science of nuclear energy materials exists in the U.S.

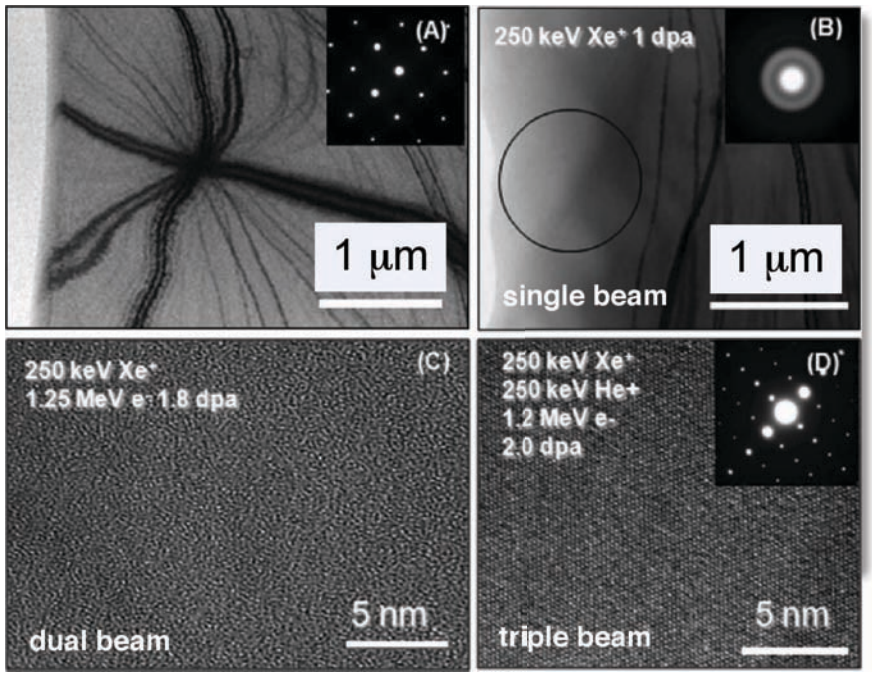

Figure 7. Triple beam irradiation shows the effects of simultaneous displacive and ionization irradiation on materials response to radiation-induced amorphization. (A) Bright-field TEM image of zircon single crystal before irradiation. (B) In-situ bright-field TEM image of zircon irradiated by 250-keV Xe^+ at room temperature (inset is an in-situ electron diffraction pattern). A completely amorphous structure can be achieved at a dose of 1 dpa for zircon irradiated with 250-keV Xe^+. (C) In-situ high resolution TEM image showing that complete amorphization was achieved at a dose of 1.8 dpa under double beam irradiation. (D) In-situ high resolution TEM image and SAED pattern showing zircon remains crystalline subjected to triple beam irradiation at a dose of 2.0 dpa. The amorphization dose increases to 4.0 dpa under triple beam irradiation. (Data obtained using the multibeam high-voltage electron microscope (HVEM) irradiation facility at Hokkaido University, Sapporo, Japan; from reference [55].)

There is no doubt that multi-ion-beam experiments can be useful in simulating the roles of hydrogen, helium, and displacement damage, and the TEM–multi-ion-beam facilities can provide a basis for the study of ionization and displacement effects that happen simultaneously in waste forms. With clever design, experiments can also be mounted to perform accelerated studies of the important vapor–liquid–solid interface. Indeed, multi-ion-beam experiments will be important in all the areas outlined for waste forms research in the ANES Workshop report[1]:

- Phase instability due to transmutation
- Helium accumulation and bubble formation
- Volume expansion from a few percent to up to 18%
- Increase in chemical reactivity and decrease in durability
- Phase separation and the formation of nano-sized inclusions associated with recoil cascades
- Increased diffusivity and transport of minority species and precipitates
- Accumulation of stored energy
- Radiation-induced amorphization

Probably the most important application of multi-ion-beam platforms is for the development of in-situ techniques that allow real-time observations of the processes extant at surfaces. Such a capability will stimulate the development of theory, simulation, and modeling using molecular dynamics, Monte Carlo, and surface physics techniques developed for other applications.

3.3. Scientific Challenge 3: Realistic modeling of radiation damage accumulation over decades, as in a nuclear energy system

Between reactor conditions and ion-beam irradiations, there is a vast area for new theory development. (Workshop discussions on this topic are summarized in Appendix H). The existing models of material degradation are not sufficiently predictive. Since it is not practicable to include all possible physical mechanisms, even a model that has been parameterized to obtain agreement with a given set of experiments has a limited range of use, e.g., interpolation within a data set and examining the dependence of critical variables. Extrapolation beyond the range of data used to fit the model is always risky. Mean-field reaction rate theory models can simulate damage accumulation over the time scales of both accelerated irradiations and reactor lifetimes, but achieve their high efficiency at a cost of losing spatial information. Moreover, even relatively complex models do not include all the relevant physical mechanisms and suffer from the need for physical parameters that may not be well specified by experiments or first-principles theory. Often, data fitting is used to try to reduce these parametric uncertainties, but such exercises typically fail to produce a unique solution. New ion-beam testing facilities would provide an opportunity for fundamental experiments to interact with theory development to minimize the uncertainty in physical parameters as well as explore relevant mechanisms.

Research groups in the U.S., Europe, and Japan are working intensely on alternative methods for predicting damage accumulations that dispense with the mean-field assumption, but the reality remains: with its unrivaled efficiency, the rate theory has been the workhorse method for material simulations for over 40 years and remains the most broadly used mesoscale material simulation method. A prudent way to go about developing new theories is to continue to use the mean-field rate theory while working on more explicit and potentially more accurate next-generation methods for simulating material degradation under irradiation. As an example, the LLNL group recently developed a new method for object Monte Carlo simulations of irradiated materials. MC methods can maintain the spatial correlations in the microstructure. The new method has already demonstrated its ability to reach simulated timescales (tens of years) and damage doses (tens of dpa) relevant for current and future reactors. This recent achievement ends the de facto monopoly of the mean-field models as the only method for material damage simulations on reactor timescales.

Development of new Object Kinetic Monte Carlo (OKMC) methods does not mean the end of using mean-field methods for simulations of irradiated materials. Both mean-field and OKMC methods are formulated in the same variables of defect cluster populations, and both cover a similarly wide range of irradiation conditions. Consequently, it is now possible to carefully examine the errors associated with the mean-field assumption employed in the rate theory, quantify the limits of the applicability of both mean-field and OKMC models, and identify ways for their mutual improvement.[56] In fact, the mean-field and the OKMC methods are likely to be the most useful for assessing candidate materials when used in combination. The same logic can be extended to other, still more accurate (and expensive) simulation methods that are currently under development, e.g., atomistic Monte Carlo. In the context of accelerated irradiation experiments, one can take advantage of the emergent diversity of simulation methods. Given their low computational cost, mean-field rate theory simulations can cover a very wide space of material testing conditions so that more expensive OKMC simulations can be focused

on one or few sets of conditions that deserve more careful theoretical analysis. Likewise, OKMC simulations can be used to further narrow the focus and to define conditions worthy of still more expensive atomistic Monte Carlo simulations. Proceeding in such a way, computational theory of irradiated materials can combine the efficiency of the existing rate theory with the accuracy of much more expensive theoretical methods. Such a multistaged theoretical approach depends on irradiations for validation, but can also be used to focus, guide, and plan further ion-beam irradiation tests.

The materials community is poised to participate in the development of new materials for advanced reactor designs by providing important scientific understanding of irradiation effects. As an example, a series of high-rate irradiation tests could be run in an ion-beam facility and the resulting data used to validate a material model or a set of material models for a well-selected target material.[57] The same models could then be used to predict the damage accumulated in the same material under significantly different irradiation conditions, e.g., at a ten-times lower dose rate and/or different temperature. Such a prediction should then be verified or contradicted in an appropriate irradiation experiment. Tried and true, small steps like this could make a significant difference and lead to discontinuous improvement in our simulation and modeling capabilities.

3.4. Scientific Challenge 4: Detailed understanding of coupled electronic and atomic dynamics on the evolution of ion-beam damage, including the combined effects of electronic and nuclear stopping

Energy transfer to the electronic structure generates electron-hole (e-h) pairs, and the nonlinear response and resulting localized electronic excitations in ceramics can lead to localized charge at defects and interfaces, rupture or changes in nature of covalent and ionic bonds, enhanced defect and atomic diffusion, and changes in phase transformation dynamics. All of these factors affect the dynamics of atomic processes and may modify or compromise the chemical, thermodynamic, and physical properties of materials.[58,59] As mentioned in our discussion of damage accumulation in waste forms, it has been observed that ionizing radiation in the presence of ion displacements leads to complex effects, among which are so-called *annealing effects*. Figure 8, an example from the literature,[60] shows that the amorphization dose (in dpa) as a function of temperature is increased by simultaneous irradiation with electrons when compared to a Xe heavy-ion alone. Additional results from ion- and electron-beam irradiation have demonstrated enhanced defect recovery[61,62] and epitaxial recrystallization rates.[63,64] A recent irradiation study[59] has shown that the stopping cross-section of slow, heavy ions predicted by the Stopping and Range of Ions in Matter (SRIM) code might be over-estimated for SiC and other compounds by a factor of two. One of the important scientific issues that would benefit from the availability of a triple ion-beam facility is improved understanding, better stopping data, and improved modeling of electronic stopping of ions in compounds,[59] which controls the energy deposition into the electronic structure.

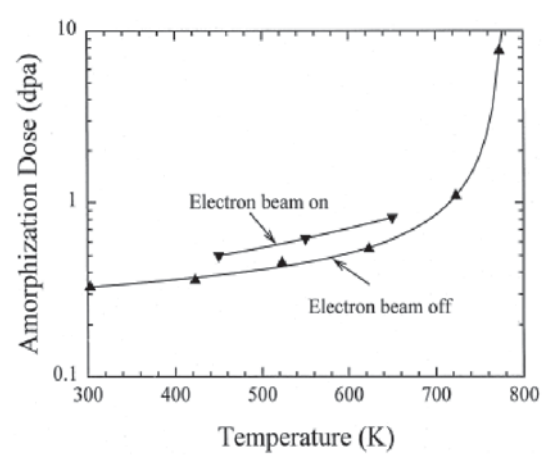

Figure 8. The critical dose for amorphization of apatite by 1.5-MeV Xe^+ with and without a simultaneous 300-keV electron beam.

Another situation where this complex and poorly understood phenomenon could play a role is in the complex evolution of nuclear fuels. Figure 9 shows results of simulations to calculate the rate of Xe ejection from a gas bubble in UO_2 during exposure to fission fragment damage under reactor conditions. The calculations show that past estimates based on simple models were in error by an order of magnitude. Additionally, they show that binary collision calculations give similar results, i.e., that thermal spikes and crystallinity effects are not important.[65]

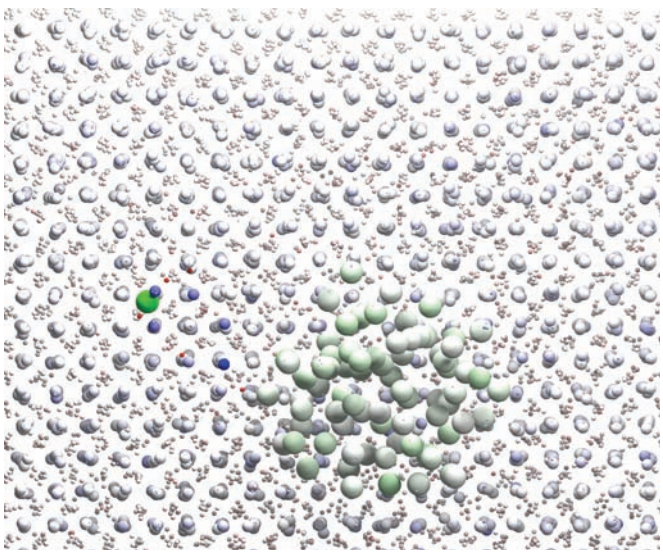

Figure 9. MD simulations showing mechanisms of fission gas bubble re-solution in UO_2 during irradiation with fission fragments.

The use of two or three beams to control implantation of gas (He^+, H^+) and damage, coupled with in-situ observation, would be a most powerful method to understand the underlying kinetic behavior and the role of electronic energy loss in this scenario.

3.5. Scientific Challenge 5: Detailed control of ion-beam synthesis and transmutation doping of nanostructures

Embedded nanostructures play a critical role in the electronics industry and in the research areas of quantum physics, quantum dots, quantum wires, and nanoscale optical materials, to mention only a few. Hence, it is not surprising that multi-ion-beam capabilities have already demonstrated a rich research frontier in an active area of technology and research.[66–75]

Potential opportunities to control synthesis processes using multiple ion beams are currently being investigated. The interaction of multiple ion beams on synthesis mechanisms provides opportunities to control the synthetic process. A good example is the synthesis of SiC nanocrystals in Si.[70] In this work, SiC nanoclusters were synthesized in Si by simultaneous dual implantation using two ion beams of C and Si ions. The authors note that the implantation is affected by excess vacancy generation by measuring the amount of synthesized SiC for simultaneous and sequential implantation. Interestingly, the multibeam simultaneous dual beam implantation is the only method to improve SiC synthesis. The authors note that the key to improved ion implantation synthesis is that the vacancies must be created in situ during C implantation to achieve enhanced output of SiC, and this is accomplished with simultaneous dual beam irradiation.

In the area of radiation-tolerant nanostructured materials, there has been pioneering research using dual ion-beams to synthesize highly uniform nanodispersoids similar to those of an ODS steel.[11] Such effects are usually produced through a combination of mechanical alloying and heat treatment. In this work, a homogeneous distribution of nano-

scale oxide particles was synthesized by applying dual ion-implantation to make a super-saturation of oxide-forming elements. Y^+ and O^+ ions were implanted (see Figure 10 and Figure 11) into a ferritic alloy at room temperature. In-situ TEM heat treatments and bulk specimen heat treatments[11] were used to refine the nanoparticles of Y_2O_3. The authors were able to conclude that dual ion implantation can induce a fine distribution of oxide-forming elements under super-saturated condition on the nanoscale, and can achieve much finer homogeneity of the nanoscale oxides compared with mechanical alloying. These results open the door to a new class of controlled experiments on nanodispersed particles for radiation tolerance.

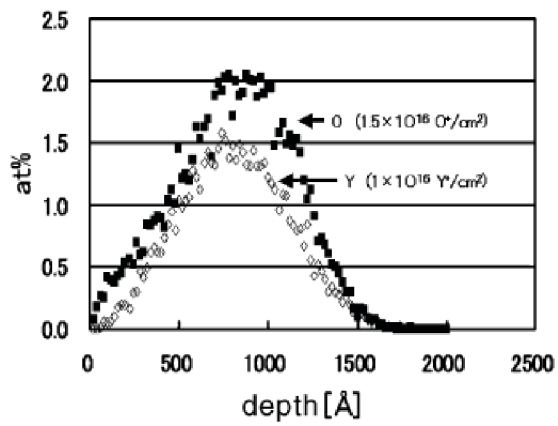

Figure 10. The calculated distribution of elements after dual ion implantation of 400-keV Y^+ and 83-keV O^+ to 1.0 x10^{16}/cm^2 and 1.5 x 10^{16}/cm^2 (from ref [11]).

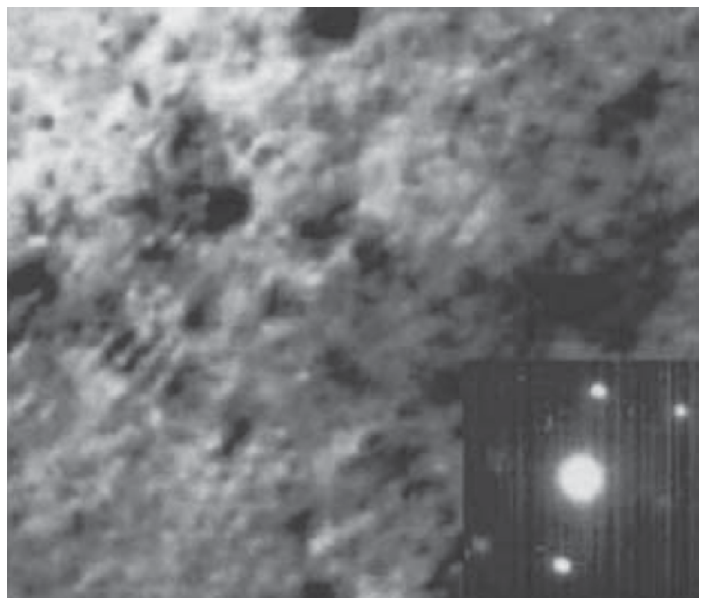

Figure 11. Nano-oxide particle structure after bulk annealing; annealed at 1073 K (from ref [11]).

3.6. Alignment with ANES Priority Research Directions

We have attempted to correlate the five scientific challenges with the Priority Research Directions in the ANES Workshop report.[1] The scientific challenges that can be addressed using a triple ion-beam facility were found to have significant impact on many of the Priority Research Directions. See Table IV.

	NANOSCALE DESIGN OF MATERIALS AND INTERFACES THAT RADICALLY EXTEND PERFORMANCE LIMITS IN EXTREME RADIATION ENVIRONMENTS	PHYSICS AND CHEMISTRY OF ACTINIDE-BEARING MATERIALS AND THE *f*-ELECTRON CHALLENGE	MICROSTRUCTURE AND PROPERTY STABILITY UNDER EXTREME CONDITIONS	MASTERING ACTINIDE AND FISSION PRODUCT CHEMISTRY UNDER ALL CHEMICAL CONDITIONS	EXPLOITING ORGANIZATION TO ACHIEVE SELECTIVITY AT MULTIPLE LENGTH SCALES	ADAPTIVE MATERIAL-ENVIRONMENT INTERFACES FOR EXTREME CHEMICAL CONDITIONS	FUNDAMENTAL THERMODYNAMIC AND KINETIC PROCESSES IN COMPLEX MULTI-COMPONENT SYSTEMS FOR FUEL FABRICATION AND PERFORMANCE	PREDICTIVE MULTISCALE MODELING OF MATERIALS AND CHEMICAL PHENOMENA IN MULTI-COMPONENT SYSTEMS UNDER EXTREME CONDITIONS
Microstructural and synergistic effects of high displacement damage coupled with implantation of transmutation products	🟢	🟡	🟢	🟡	🟢	🟡	🟡	🟢
Evolution of microstructure, physical, and chemical properties in complex actinide fuels and nuclear waste management materials	🟢	🔴	🟢	🟡	🟢	🟡	🟡	🟢
Realistic modeling of radiation damage accumulation over decades, as in a nuclear energy system	🟢	🟡	🟢	🔴	🟢	🟡	🟡	🟢
Detailed understanding of coupled electronic and atomic dynamics on the evolution of ion-beam damage, including the combined effects of electronic and nuclear stopping	🟢	🟢	🟢	🟡	🟡	🟢	🟢	🟢
Detailed control of ion-beam synthesis and transmutation doping of nanostructures	🟢	🟡	🟢	🔴	🟡	🟡	🟡	🟢

Table IV. Correlation of scientific challenges with Priority Research Directions. 🟢 = well correlated, 🟡 = partially correlated, 🔴 = uncorrelated. The five scientific challenges are distilled from a longer list in Appendix F.

4. Technical Benefits

4.1. Impact on fission and fusion energy sciences

This workshop was useful for "feeling the pulse" of the radiation materials community and gauging its readiness for a major push to reenergize materials R&D for nuclear energy. The community has shrunk over the past 20 years, in part because of steady reductions in funding and a generally negative public perception of nuclear energy. It was noted that to certify materials for new reactor designs, regulators have always relied—and must continue to rely—on incomplete data and models of material performance. The ability of a given candidate material to sustain its functions over a lifetime in the reactor can be fully assessed only after the reactor is already built and has served for its expected long lifetime. At the same time, it is the unknown limits of material performance that constrain material development for future reactor designs. To be useful, new cycles in materials development have to be as short as possible while still reliably simulating reactor conditions as closely as possible.

For materials research and development, the research community must develop reliable data from materials irradiation experiments, data that have been obtained under a wide range of conditions and supported by carefully validated materials models based on accurate materials theory. Mechanisms of material degradation in the reactor environment are many, they are complex, and they compete with each other. The key science challenge is to demonstrate that it is possible to understand all the relevant mechanisms and to develop quantitative theory to accurately predict their interactions over the reactor timescales. New, advanced materials developed through ion-beam research can become enablers for advanced fission and fusion reactors.

The consensus from workshop attendees was that accelerated ion-beam materials experiments can and should play an important role in the current push to undertake the fundamental science of ANES. The few still-existing facilities can be upgraded and new facilities can be deployed quickly and at a low cost. By their nature, ion-beam facilities are nimble, allowing for numerous short experiments under a wide variety of testing conditions. They are perfect for exploratory research on different classes of materials, for initial material screening, and for guiding and focusing much costlier and slower experiments, such as neutron source tests. Triple-beam accelerator facilities are essential for simulating conditions relevant to fast-spectrum fission (to simulate fuels irradiation conditions, e.g., fission track damage concurrent with fission gas buildup) and fusion reactors. Such facilities also can provide a convenient platform for the entire radiation materials community. There is value in establishing a triple-beam capability close to material synthesis and characterization capabilities located in one center. However, because materials irradiated by ions are in most instances nonradioactive, they can readily be shipped, allowing much material synthesis and most pre- and post-irradiation material characterization to take place elsewhere. Consequently, a new ion-beam facility would mesh well with the current U.S. network of materials research facilities.

A typical ion-beam experiment will use high particle fluxes to impart the same degree of damage as a material would receive over its lifetime in a reactor. What remains to be determined is whether the damage a material accumulates during a short (days or less) ion beam irradiation can be used to predict the behavior of the material over the much longer lifetime of a reactor. The premise of using ion-beam facilities for accelerated irradiations is that materials theory and simulations can provide

a reliable connection between accelerated experiments and material lifetime predictions. One of the most important measures of success for an accelerated testing program will be whether materials performance models validated against accelerated irradiation experiments are accepted for material certification in future reactor designs. Time and a commitment to the basic science will tell us if this approach is valid.

4.2. Training and supporting the energy scientists of the future

Participants also pointed out the importance of a triple ion-beam facility in training the next generation of scientists. Irradiation damage experiments at neutron sources can be quite time consuming, often entailing timeframes that are inconsistent with that of a Ph.D. First, sample space in neutron sources is quite precious and can be difficult to obtain. Second, irradiations can take months or years to reach desired doses. Finally, samples are often radioactive when removed from the neutron source and need to cool for months before experiments can be carried out. Ion irradiation has the advantages of high dose rates, low cost for high-dose experiments, and no activation, so experiments can be carried out very efficiently. Samples can be studied in situ or immediately after irradiation and treated similarly to those that are nonirradiated or, at worst, have very low activity.

4.3. Impact beyond advanced nuclear energy systems

Workshop participants also described scientific challenges in an area of basic physics and materials science problems related to synthesis of new materials using co-irradiation/implantation. This constitutes a broader area of interest than that related to reactor, accelerator, or nuclear waste technologies. Energetic ions can be used to modify or synthesize new materials through processes such as implantation, disordering, or phase transformations. While this discussion is outside the scope of the current report, we point to a small but growing community (currently primarily outside the U.S.) that could make use of a high-energy (MeV) triple ion-beam irradiation facility.[66–75]

4.4. Feasibility of a triple beam accelerator as a national user facility

A triple ion-beam national user facility[76,77] would inherently differ from a reactor or a light source because those types of facilities incorporate significant volume and geometry to accommodate multiple users simultaneously. A potential issue with a triple ion-beam facility is that two or three ion-beam accelerators can be allocated to one experiment, leaving other users to wait while samples are “processed” in sequence, one at a time. However, this facility is closer in character to the BES Electron Beam Microcharacterization Centers[78] than to a light source. Although single-user facilities can never realize the growth in user base of a light source, they have been demonstrated to be successful and important to the scientific community.

Perhaps a more relevant example to this discussion is that of the Center for Accelerator Mass Spectrometry (CAMS) at LLNL. CAMS, while not a formal national user facility, is based around a 10 MV FN tandem accelerator and provides accelerator mass spectrometry and ion beam analysis/materials modification capabilities to LLNL, government agencies, and other clientele. CAMS has an outstanding record of outreach and currently has over 100 university, DOE, and private sector collaborations. In addition, CAMS has hosted over

1000 faculty and student visitors in the past decade, resulting in more than 125 Masters and Ph.D. theses. These interactions have led to an outstanding, broad scientific impact with CAMS scientists authoring 18 and 13 percent of LLNL's *Science* and *Nature* articles, respectively, over the past decade. CAMS research has been featured on the covers of ten journals in the past five years.

We believe that a triple ion-beam national user facility is both feasible and desirable.

5. Facility Specifications to Meet Scientific Needs

Discussion among participants (comments are summarized in Appendix I) led to the consensus that two types of simultaneous multiple beam systems would be needed:

System 1: A thin-film implantation system based around a TEM and one or more simultaneous ion beams to implant/irradiate specimens less than one micrometer thick

System 2: A simultaneous triple ion-beam (heavy ions, He, and H) irradiation system for producing uniformly implanted/irradiated specimens ranging in thickness from several hundred nanometers up to several micrometers

Workshop participants gave their input concerning desired capabilities for each system. Table V provides a summary of these suggestions that bound the phase-space for each system. The table is not intended to be a specification sheet; rather, it outlines what should be considered in each system in terms of ion beam/accelerator configuration and requirements for the target chamber for in-situ analysis and diagnostics.

System 1 will require a facility to be constructed around a TEM for online monitoring of the ion-beam irradiations to take proper advantage of TEM capabilities. Use of a TEM necessitates use of thin (<1 μm thick) materials for irradiation. With this system, the overriding design factor will be to construct ion-beam transport capabilities that will be compatible with the TEM. Owing to the thin-film nature of samples to be implanted/irradiated, ion-beam energies will be relatively low, and a variety of small, low-energy accelerators (1–3 MV terminal potential) with an appropriate ion source (such as an ECR source) can likely fulfill implantation needs. Such accelerators could also enable the use of in-situ ion-beam analysis monitoring techniques (i.e., Rutherford backscattering spectroscopy, nuclear reaction analysis, and elastic recoil detection). However, a thin-film implantation system will likely yield potential surface effects arising from the implants producing dpa, He, and/or H profiles very near to the material's surface.

TEM with in-situ ion irradiation has obvious advantages, including viewing and measuring the development of microstructure in "real time" at temperature, under strain, with dose and to high dose, etc. Mechanisms can be observed and measured for the first time, as documented in recent papers on ferritic Fe and Fe-Cr model alloys.[79] In-situ TEM and irradiation of thin samples, using variations in foil thickness as a parameter, can be used as critical experimental benchmark tests of simulation codes of neutron irradiation to high dose.[80] A next-

generation in-situ irradiation/TEM facility could use the expanded gap of an aberration-corrected scope to "easily" include 2–3 ion beams. The compromise to high resolution probably will not be important; dark-field weak-beam electron microscopy is far more useful than images of atoms. The enhanced resolution for energy-filtered transmission electron microscopy would be very useful. Ion beams' incidence at or near 30 degrees to the electron beam is probably essential to in-situ, real-time observations.

System 2 will require a facility that can produce both shallow and deep implants and, by varying the incident ion-beam energies, volumetric implants/irradiations that are at least several micrometers thick. These capabilities will be necessary to overcome surface effects, to produce samples with implant depths that approach the grain size of many candidate materials, and to produce "bulk" samples for post-irradiation materials experimentation and characterization. With such a system, online TEM analysis will be precluded for candidate samples over 1 μm thick. To produce such samples, System 2 will require at least one accelerator capable of producing heavy ions with energies of least several tens of MeV (and preferably close to 100 MeV) to enable heavy ion implants deep into candidate materials. Such high-energy ions are also important to mimic energy deposition and damage processes of fission products. Accelerators, such as a FN tandem or cyclotron, that can produce up to 100-MeV heavy ions with μA beam currents for the majority of ions with Z >10, are well-placed to be cornerstones of such a facility. Such accelerators can also meet the requirement, expressed by some participants, of performing H^+ and He^+ ion implants to >0.1-mm depths in candidate materials.

In addition to the heavy ion accelerator, the accelerators for System 2 that produce hydrogen and helium beams should have sufficient terminal potentials to produce hydrogen and helium implants that at least match the depth of the heavy ion implant. This capability will enable use of in-situ ion-beam analysis monitoring techniques (i.e., RBS) as well as performance of simultaneous irradiations. This requirement implies accelerators that can produce hydrogen beams with energies up to ~5 MeV and helium beams with energies up to ~20 MeV. The target chamber design for System 2 can likely be more flexible than for System 1, as there is no need to accommodate TEM. It is not difficult to envision interchangeable target chambers in System 2 to accommodate specific irradiation monitoring needs.

System 1 Requirements	Driver
Heavy (3 < Z < 90) ions (1 < E < 25 MeV) 0.1 to 5 particle μA currents	dpa production (1 to 150 dpa)
Protons (0.1< E < 1 MeV) 0.1 to a few particle μA currents	Hydrogen implantation to atomic part per thousand levels
Helium (0.1< E < 3 Mev) 0.1 to a few particle μA currents	Helium implantation to atomic part per thousand levels
Ion clusters (<300 keV) (desirable but not essential)	Cluster and surface effects
Electron gun (E < 100 keV) μA to 20 mA currents	Tease apart displacement damage from ionization damage
TEM with sufficient energy to traverse thin film	In-situ monitoring of implant
Irradiation area, 3 x 3 mm to 2 x 2 cm	Post-implantation analysis requirement
Goniometer with 3Z + 3q degrees of freedom	Sample manipulation, positioning, and ion channeling
Precise (within 5 °C) temperature control (-269 < T < 1000 °C)	Basic materials science of materials damage
Simultaneous delivery of up to 2 ion beams with in-situ TEM	Basic materials science of materials damage
In-situ nanoindentation properties (desirable but not essential)	Material properties under irradiation
Ability to irradiate actinide oxides	Fuel properties under damage
In-situ straining stage	Mechanical properties of thin films
In-situ ion-beam analysis (IBA) (RBS, ERDA, NRA, channeling)	Materials characterization during and post-irradiation
Vacuum <10^{-7} Torr and infrared camera to monitor sample temperature	Irradiation diagnostics

System 2 Requirements	Driver
Heavy (3 < Z < 90) ions (1 < E < 25 MeV),0.1 to 5 particle μA currents	dpa production (1 to 150 dpa) for bulk properties
Protons (0.1 < E < 5 MeV) 0.1 to 2 particle μA currents	Hydrogen implantation up to 100 μm deep for bulk properties
Helium (1 < E < 20 Mev) 0.1 to 2 particle μA currents	Helium implantation up to 100 μm deep for bulk properties
Electron gun (10 < E < 100 keV) μA to 20 mA currents	Tease apart displacement damage from ionization damage
Irradiation area, 3 x 3 mm to 2 x 2 cm	Post-implantation analysis requirement
Precise (within 5 °C) temperature control (-180 < T < 1000 °C)	Simulation of reactor environment
Simultaneous delivery of up to three ion (heavy, H, He) beams	Synergistic effects
Demonstrated ability for 24h/7 day accelerator operations	High dpa, low dpa rate experiments
In-situ nanoindentation properties (desirable but not essential)	Material properties under irradiation
Ability to irradiate actinide oxides	Materials properties of aged fuel
In-situ ion beam analysis (IBA)	Materials characterization during and post irradiation
Ability to vary ion beam energy to produce volumetric implants	Macroscopic "bulk" sample" for post-irradiation experimenting
Vacuum <10^{-7} Torr and Thermal camera to monitor sample temperature	Irradiation diagnostics

Note 1: 1 particle μA = 6.25 x 10^{12} particles /second.

Note 2: Ability to reproduce heavy ions beams for the majority of the periodic table is highly desirable.

Table V. Facility requirements for the two triple-beam systems. System 1: Thin-film implantation system based around a TEM and one or more simultaneous ion beams to implant specimens up to 1 μm thick. System 2: Simultaneous triple ion-beam (heavy, H, and He) irradiation system for production of uniformly implanted specimens ranging from several hundred nanometers up to several micrometers thick.

6. Projected Characteristics of the User Community at a High-Energy (MeV) Triple Ion-Beam Irradiation Facility

Workshop organizers solicited information from participants as well as a broader community identified by colleagues and DOE program managers. Thirty-six responses were collected and tabulated. No responses from LLNL were included in the summary below.

Figure 12 indicates that by a broad margin, those surveyed were interested in becoming part of a U.S. community associated with a high-energy (MeV) triple ion-beam irradiation facility.

Would you want to be part of a US community for such a facility?

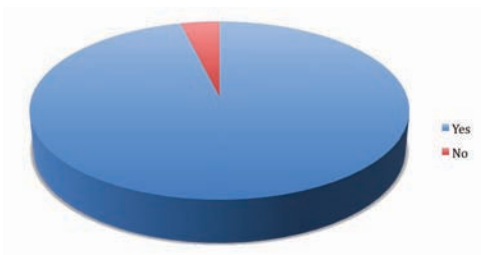

Figure 12. Those surveyed were interested in being part of the scientific community associated with a three-beam accelerator.

Participants projected 229 potential users from eight states and one foreign country. Nearly half of the users of such a facility are expected to come from DOE laboratories. Universities are expected to comprise about 28% of the user community (Figure 13).

Use by institution Type

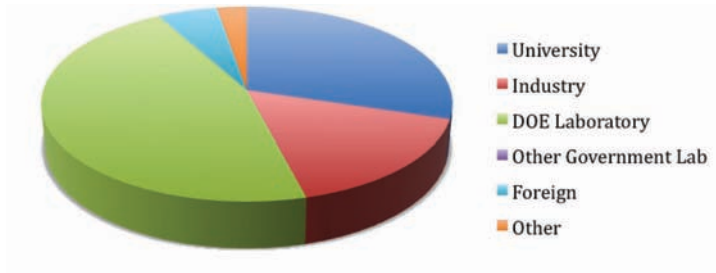

Figure 13. Projected use by institution type.

Potential users project that the user employment level will be about equally split between postdoctoral associates and professionals (Figure 14). Participants projected an initial usage of 217 8-hour shifts per year.

User employment level

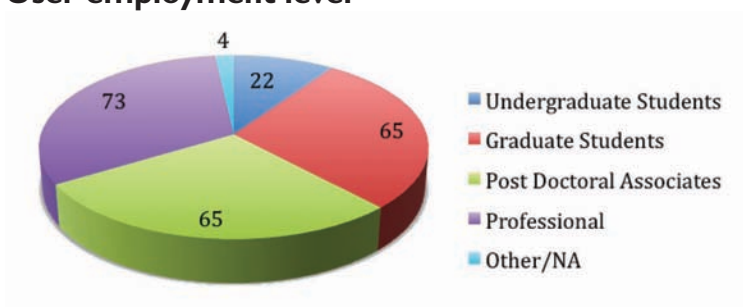

Figure 14. Projected user employment level. The numbers reflect the absolute number of projected users provided by those responding to the survey.

Materials science will be the predominant scientific discipline using a high-energy triple ion-beam irradiation facility (Figure 15).

User employment level

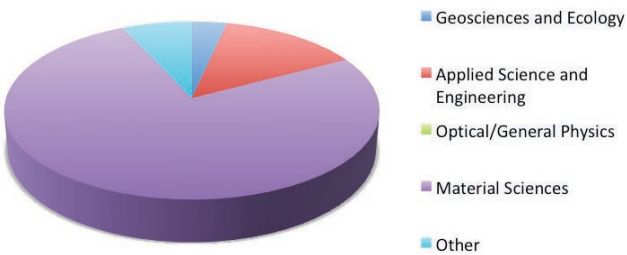

Figure 15. Projected Users by Discipline.

Figure 16 illustrates the projected split of types of research among nonproprietary, nonproprietary and proprietary, and proprietary only. This survey predicts a significantly larger fraction of nonproprietary and proprietary research than for BES Light Sources in FY 2008.

Nature of Research

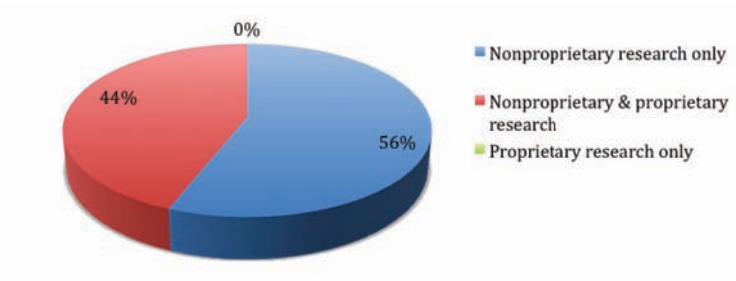

Figure 16. Projected split of research types between nonproprietary and proprietary.

It is projected that support for the science studied using the triple ion-beam irradiation facility will be dominated by research funded by BES and NE (Figure 17). The fourth-largest supporter is projected to be FES.

Source of User Support

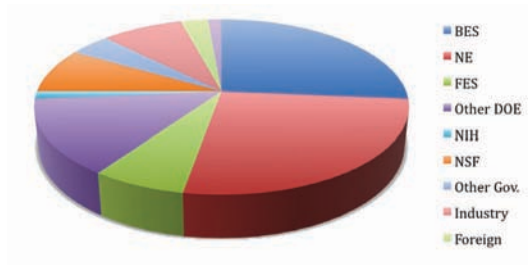

Figure 17. Projected sources of support for research on a high-energy triple ion-beam irradiation facility.

A significant outcome of this workshop was the realization that there is interest in three types of experiments: (1) experiments with in-situ capabilities, (2) in-situ real-time experiments using electron microscopy, and (3) post-irradiation experiments. Seventy-seven percent of experiments will employ accelerators, target chambers, and a variety of standard ion-beam analysis capabilities. About a quarter of experiments will use in-situ irradiations in an electron microscope (see Figure 18).

Class of Experiments

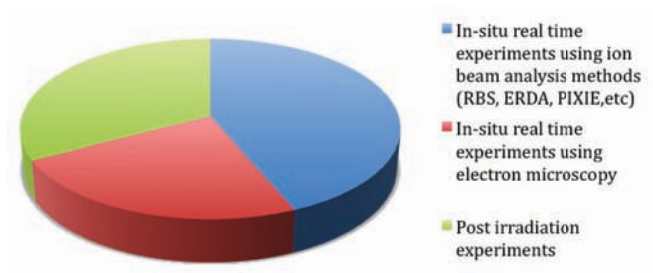

Figure 18. Projected needs for in-situ and post-irradiation experiments.

Irradiation experiments carried out at a high-energy triple ion-beam irradiation facility will require extensive post-irradiation characterization or correlation with neutron irradiation. Respondents indicated that they would make extensive and broad use of BES and other scientific user facilities as part of their experimental plan. Their projections are detailed in Table VI.

Other facilities that may be used with this facility	
Stanford Synchrotron Radiation Laboratory (SPEAR3)	1.39%
National Synchrotron Light Source (BNL)	4.17%
Advanced Light Source (LBNL)	6.94%
Advanced Photon Source (ANL)	11.11%
Linac at SLAC	0.00%
Linac Coherent Light Source (SLAC)	1.39%
National Synchrotron Light Source II (BNL)	4.17%
Manuel Lujan, Jr. Neutron Scattering Center (LANL)	6.94%
High Flux Isotope Reactor (ORNL)	8.33%
Spallation Neutron Source (ORNL)	4.17%
Electron Microscopy Center for Materials Research (ANL)	12.50%
National Center for Electron Microscopy (LBNL)	8.33%
Shared Research Equipment Program (ORNL	6.94%
Center for Nanophase Materials Sciences (ORNL)	2.78%
Molecular Foundry (LBNL)	1.39%
Center for Integrated Nanotechnologies (SNL & LANL)	8.33%
Center for Functional Nanomaterials (BNL)	1.39%
Center for Nanoscale Materials (ANL)	4.17%
ATR National Scientific User Facility	5.56%

Table VI. Percentage of respondents who indicated that they would use other facilities in conjunction with a high-energy triple ion-beam irradiation facility.

7. Recommendations and Conclusions

1. A clear statement was made of the role that ion beams play in advancing our fundamental knowledge of irradiation effects. *Ion beams are invaluable because they provide a research platform for investigating the fundamental mechanism underpinning radiation effects in ANESs. They provide control of variables that will allow investigation of unit mechanisms.* Therefore, part of this report is dedicated to laying out the basic research that would be catalyzed by the existence of a U.S. triple ion-beam facility.

2. The community is strongly interested in experiments where mechanisms can be probed in real time, in situ. This includes the usual ion-beam techniques (channeling, PIXE, ERDA, RBS, etc.) and in-situ, multiple-ion-beam irradiation in the electron microscope.

3. Theory, simulation, and modeling will play a central role in the understanding of data generated at a triple ion-beam facility. Damage effects due to ion beams can be realized three orders of magnitude faster than those occurring in ANESs, allowing high-dose effects to be studied in realistic timeframes. Experimental comparisons with theoretical predictions as a function of variables such as energy, temperature, and dose rate will provide critical tests of our understanding of the unit mechanisms and our ability to bridge time and length scales using modeling and simulation.

4. A triple ion-beam facility would play an important role in training the scientific leaders of the future. Irradiation damage experiments at neutron sources can last for a long time, having timeframes that are inconsistent with that of a doctoral graduate student's matriculation. Additionally, sample space in neutron sources is quite precious and can be difficult to obtain. Irradiations can take months or years to reach desired doses. Finally, samples are often radioactive when removed from the neutron source and need to cool for months before experiments can be carried out. In contrast, ion irradiation has the advantage of high displacement and simulated "transmutation" rates with *no activation*. Experiments can be carried out very efficiently and samples can be characterized in situ or immediately after irradiation.

5. While the original intent of this workshop was to look into a triple ion-beam accelerator facility, it became clear that the community also needs another highly complementary capability: one or two ion beams coupled with a next-generation electron microscope. It was not possible to give this topic the attention that it deserves in this report. A separate workshop should take an in-depth look into the research needs for a facility where ion beams are interfaced with an electron microscope.

8. References

[1] J. Roberto, T. Diaz de la Rubia, Basic Research Needs For Advanced Nuclear Energy Systems: Report of the Basic Energy Sciences Workshop on Basic Research Needs for Advanced Nuclear Energy Systems, Office of Basic Energy Sciences, Germantown, MD

[2] A. Möslang, Existing and Future Irradiation Facilities: Their Availability and Access, Nuclear Science Structural Materials for Innovative Nuclear Systems SMINS: Workshop Proceedings, vol. 2007, OECD Nuclear Energy Agency, Karlsruhe, Germany, 2007. pp. http://www.nea.fr/html/science/struct_mater/Presentations/MOESLANG.pdf.

[3] T. Tanaka, K. Oka, S. Ohnuki, S. Yamashita, T. Suda, S. Watanabe, E. Wakai, Synergistic effect of helium and hydrogen for defect evolution under multi-ion irradiation of Fe-Cr ferritic alloys, Elsevier Science Bv, Kyoto, Japan, 2003. pp.294.

[4] G. R. Odette, M. J. Alinger, B. D. Wirth, Recent developments in irradiation-resistant steels, Ann. Rev. Mater. Res. 38 (2008) 471.

[5] T. R. Allen, J. Gan, J. I. Cole, M. K. Miller, J. T. Busby, S. Shutthanandan, S. Thevuthasan, Radiation response of a 9 chromium oxide dispersion strengthened steel to heavy ion irradiation, Journal of Nuclear Materials 375 (2008) 26.

[6] J. Gan, T. R. Allen, R. C. Birtcher, S. Shutthanandan, S. Thevothasan, Radiation effects on the microstructure of a 9Cr-ODS alloy, JOM 60 (2008) 24.

[7] E. Horowitz, Asme, The Importance Of Establishing An Operational Approach For The Selection Of Materials In The Reactors Of The Future, Orlando, FL, 2008. pp.405.

[8] R. Lasser, E. Diegele, J. L. Boutard, A. Peacock, The long term development of fusion materials in the EU: achievements and open issues, Sibiu, Romania, 2007. pp.727.

[9] E. A. Marquis, Core/shell structures of oxygen-rich nanofeatures in oxide-dispersion strengthened Fe-Cr alloys, Applied Physics Letters 93 (2008).

[10] M. A. Pouchon, J. Chen, C. Degueldre, A. Froidevall, H. Emerich, W. Van Beek, EXAFS study on irradiated ODS ferritic steel, In: Y. W. Chang, N. J. Kim, C. S. Lee, (Eds), Cheju Isl, South Korea, 2007. pp.1761.

[11] S. Sakuma, S. Yamashita, K. Oka, S. Ohnuki, L. E. Rehn, E. Wakai, Y_2O_3 nano-particle formation in ODS ferritic steels by Y and O dual ion-implantation, Elsevier Science Bv, Kyoto, Japan, 2003. pp.392.

[12] M. Samaras, M. Victoria, W. Hoffelner, Nuclear Energy Materials Prediction: Application Of The Multi-Scale Modeling Paradigm, Nuclear Engineering and Technology 41 (2009) 1.

[13] H. B. G. Casimir, On Onsager's principle of microscopic reversibility, Rev. Mod. Phys. 17 (1945) 343.

[14] S. R. d. Groot, P. Mazur, Non-equilibrium thermodynamics, Dover Publications, New York, 1984.

[15] L. Onsager, Reciprocal relations in irreversible processes. I, Phys. Rev. 37 (1931) 405.

[16] L. Onsager, Reciprocal relations in irreversible processes. II, Phys. Rev. 38 (1931) 2265.

[17] I. Prigogine. Etude thermodynamique des phenomenes irreversibles. Dunod, Paris, 1947.

[18] E. P. Wigner, Derivations Of Onsager Reciprocal Relations, J. Chem. Phys. 22 (1954) 1912.

[19] G. Martin, Phase-Stability Under Irradiation - Ballistic Effects, Phys. Rev. B 30 (1984) 1424.

[20] G. Martin, P. Bellon, Driven alloys, Solid State Physics - Advances in Research and Applications, vol. 50, Academic Press Inc, San Diego, 1997. pp.189.

[21] J. Ye, P. Bellon, R. A. Enrique, Nanoscale patterning of composition and chemical order induced by displacement cascades in irradiated alloys, Elsevier Science Bv, Pacific Grove, CA, 2004. pp.265.

[22] M. J. Demkowicz, R. G. Hoagland, J. P. Hirth,

Interface structure and radiation damage resistance in Cu-Nb multilayer nanocomposites, Physical Review Letters 100 (2008) 4.
[23] G. S. Was, Fundamentals of radiation materials science metals and alloys, Springer, Berlin, 2007.
[24] Y. Serruys, P. Trocellier, S. Miro, E. Bordas, M. O. Ruault, O. KaÔtasov, S. Henry, O. Leseigneur, T. Bonnaillie, S. Pellegrino, S. Vaubaillon, D. Uriot, JANNUS: A multi-irradiation platform for experimental validation at the scale of the atomistic modeling, Journal of Nuclear Materials 386-388 (2009) 967.
[25] M. B. Lewis, W. R. Allen, R. A. Buhl, N. H. Packan, S. W. Cook, L. K. Mansur, Triple Ion-Beam Irradiation Facility, Nucl. Instrum. Methods Phys. Res. Sect. B-Beam Interact. Mater. Atoms 43 (1989) 243.
[26] L. K. Mansur, E. H. Lee, M. B. Lewis, S. J. Zinkle, Applications of Multiple-Ion Irradiations to Metals, Ceramics, and Polymers, In: J. A. E. R. Institute, (Ed), Proceedings of the International Conference on Evolution in Beam Applications, Radiation Application Development Association, Tokai-mura, Japan, Takasaki, Japan, 1991.
[27] Y. Serruys, M. O. Ruault, P. Trocellier, S. Henry, O. Kaitasov, P. Trouslard, Multiple ion beam irradiation and implantation: JANNUS project, Elsevier Science Bv, Paris, France, 2004. pp.124.
[28] F. A. Garner, Impact Of The Injected Interstitial On The Correlation Of Charged-Particle And Neutron-Induced Radiation-Damage, Journal of Nuclear Materials 117 (1983) 177.
[29] E. H. Lee, L. K. Mansur, M. H. Yoo, Spatial variation in void volume during charged particle bombardment -- the effects of injected interstitials, Journal of Nuclear Materials 85-86 (1979) 577.
[30] http://www.igcar.ernet.in/igc2004/igcanr2006.pdf
[31] Y. Kohno, K. Asano, A. Kohyama, K. Hasegawa, N. Igata, New Dual-Ion Irradiation Station At The University Of Tokyo, Journal of Nuclear Materials 141 (1986) 794.
[32] M. Iseki, Y. Kizuka, S. Mori, K. Kohmura, M. Kiritani, Recoil energy spectrum effect in vanadium by electron and light- and heavy-ion irradiation, Elsevier Science Bv, Obninsk, Russia, 1995. pp.492.
[33] H. Tyrroff, W. Neumann, B. Richter, Strahlkopplung von Tandetron-beschleuniger und Ionenimplanter zur Durchfürhung von Mehrstrahlexperimenten im Forschungzentrum Rossendorf, Forschungzentrum Rossendorf, FZR-308.
[34] W. Wesch, A. Kamarou, E. Wendler, K. Gartner, P. I. Gaiduk, S. Klaumunzer, Ionisation stimulated defect annealing in GaAs and InP, Elsevier Science Bv, Kobe, Japan, 2002. pp.1018.
[35] A. Kohyama, Y. Katoh, M. Ando, K. Jimbo, A new Multiple Beams-Material Interaction Research Facility for radiation damage studies in fusion materials, Elsevier Science Sa, Rome, Italy, 1999. pp.789.
[36] S. Hamada, Y. Miwa, D. Yamaki, Y. Katano, T. Nakazawa, K. Noda, Development of a triple beam irradiation facility, Elsevier Science Bv, Sendai, Japan, 1997. pp.383.
[37] B. P. Il'enko, I. N. Onishchenko, V. L. Pershin, Accelerator Of Combined Heavy And Light Ion Beams, Probl. At. Sci. Tech. (2008) 33.
[38] N. Yu, M. Nastasi, T. E. Levine, J. R. Tesmer, M. G. Hollander, C. R. Evans, C. J. Maggiore, In-Situ Capability Of Ion-Beam Modification And Characterization Of Materials At Los Alamos National Laboratory, Elsevier Science Bv, Denton, TX, 1994. pp.566.
[39] H. Tsuchida, H. Takahashi, In situ observation of austenitic stainless steels during dual-beam irradiation, Elsevier Science Bv, Honolulu, HI, 1995. pp.112.
[40] C. W. Allen, E. A. Ryan, An Hitachi H-9000 for Argonne's HVEM-Tandem facility: Expanded capacities for in situ ion beam studies, Hitachi Instrument News, 1996. pp.3.

[41] http://www.ganil.fr/ciril/gdr/pleniere.html
[42] H. Abe, H. Naramoto, K. Hojou, S. Furuno, The TEM-accelerators facility at JAERI-Takasaki and its application to materials science, JAERI Research 96-047.
[43] K. Hojou, S. Furuno, K. N. Kushita, H. Otsu, K. Izui, Insitu Observation Of Damage Evolution In SiC Crystals During He^{+} And H^{+2} Dual-Ion Beam Irradiation, Elsevier Science Bv, Clearwater, FL, 1991. pp.583.
[44] Y. Serruys, M. O. Ruault, P. Trocellier, S. Miro, A. Barbu, L. Boulanger, O. Kaietasov, S. Henry, O. Leseigneur, P. Trouslard, S. Pellegrino, S. Vaubaillon, JANNUS: experimental validation at the scale of atomic modeling, C. R. Phys. 9 (2008) 437.
[45] BESAC, Directing Matter and Energy: Five Challenges for Science and the Imagination A Report from the Basic Energy Sciences Advisory Committee, U.S. Department of Energy, Germantown, MD
[46] J. Wadsworth, G. W. Crabtree, R. J. Hemley, Basic Research Needs For Materials Under Extreme Environments, in: Basic Research Needs Workshop Reports, Office of Basic Energy Sciences, Germantown, MD, February 2008
[47] N. Sekimura, T. Iwai, Y. Arai, S. Yonamine, A. Naito, Y. Miwa, S. Hamada, Synergistic effects of hydrogen and helium on microstructural evolution in vanadium alloys by triple ion beam irradiation, Elsevier Science Bv, Colorado Springs, Colorado, 1999. pp.224.
[48] Y. Guerin, G. S. Was, S. J. Zinkle, Materials Challenges for Advanced Nuclear Energy Systems, MRS Bull. 34 (2009) 10.
[49] S. X. Wang, B. D. Begg, L. M. Wang, R. C. Ewing, W. J. Weber, K. V. G. Kutty, Radiation stability of gadolinium zirconate: A waste form for plutonium disposition, J. Mater. Res. 14 (1999) 4470.
[50] F. A. Garner, E. P. Simonen, B. M. Oliver, L. R. Greenwood, M. L. Grossbeck, W. G. Wolfer, P. M. Scott, Retention of hydrogen in fcc metals irradiated at temperatures leading to high densities of bubbles or voids, Elsevier Science Bv, Thun, Switzerland, 2005. pp.122.
[51] J. D. Hunn, E. H. Lee, T. S. Byun, L. K. Mansur, Helium and hydrogen induced hardening in 316LN stainless steel, Journal of Nuclear Materials 282 (2000) 131.
[52] J. D. Hunn, M. B. Lewis, E. H. Lee, Hydrogen Retention in Ion-Irradiated Steels, Proc. 2nd International Topical Meeting on Nuclear Applications of Accelerator Technology, American Nuclear Society Inc, La Grange Park, Illinois, 1998. pp.375.
[53] E. Wakai, K. Kikuchi, S. Yamamoto, T. Aruga, M. Ando, H. Tanigawa, T. Taguchi, T. Sawai, K. Oka, S. Ohnuki, Swelling behavior of F82H steel irradiated by triple/dual ion beams, Elsevier Science Bv, Charleston, South Carolina, 2002. pp.267.
[54] C. Guéneau, S. Chatain, J. C. Dumas, J. Lechelle, C. Rado, F. Defoort, N. Dupin, B. Sundman, H. Noel, R. Konings, FUELBASE: A Thermodynamic Database For Advanced Nuclear Fuels, Proceedings HTR2006: 3rd International Topical Meeting on High Temperature Reactor Technology, HTR2006, Johannesburg, South Africa, 2006.
[55] J. Lian, L. M. Wang, K. Sun, R. C. Ewing, In Situ TEM of Radiation Effects in Complex Ceramics, Microsc. Res. Tech. 72 (2009) 165.
[56] R. E. Stoller, S. I. Golubov, C. Domain, C. S. Becquart, Mean field rate theory and object kinetic Monte Carlo: A comparison of kinetic models, Elsevier Science Bv, Orlando, FL, 2007. pp.77.
[57] G. S. Was, J. T. Busby, T. Allen, E. A. Kenik, A. Jenssen, S. M. Bruemmer, J. Gan, A. D. Edwards, P. M. Scott, Emulation of neutron irradiation effects with protons: validation of principle, Journal of Nuclear Materials 300 (2002) 198.
[58] N. Itoh, A. M. Stoneham. Materials modification by electronic excitation. Cambridge University Press, Cambridge, UK ; New York, NY, 2001.

[59] Y. Zhang, I.-T. Bae, K. Sun, C. Wang, M. Ishimaru, Z. Zhu, W. Jiang, W. J. Weber, Damage profile and ion distribution of slow heavy ions in compounds, Journal of Applied Physics 105 (2009) 104901.

[60] R. Devanathan, K. E. Sickafus, W. J. Weber, M. Nastasi, Effects of ionizing radiation in ceramics, Elsevier Science Bv, Cincinnati, Ohio, 1997. pp.113.

[61] W. J. Weber, L. M. Wang, Y. W. Zhang, W. L. Jiang, I. T. Bae, Effects of dynamic recovery on amorphization kinetics in 6H-SiC, Caen, France, 2007. pp.2793.

[62] Y. Zhang, J. Lian, C. M. Wang, W. Jiang, R. C. Ewing, W. J. Weber, Ion-induced damage accumulation and electron-beam-enhanced recrystallization in $SrTiO_3$, Phys. Rev. B 72 (2005).

[63] I. T. Bae, W. J. Weber, M. Ishimaru, Y. Hirotsu, Effect of ionization rates on dynamic recovery processes during electron-beam irradiation of 6H-SiC, Applied Physics Letters 90 (2007).

[64] I. T. Bae, Y. W. Zhang, W. J. Weber, M. Higuchi, L. A. Giannuzzi, Electron-beam induced recrystallization in amorphous apatite, Applied Physics Letters 90 (2007).

[65] D. Schwen, M. Huang, P. Bellon, R. S. Averback, Molecular dynamics simulation of intragranular Xe bubble re-solution in UO2, Journal of Nuclear Materials In Press, Corrected Proof (2009).

[66] H. Bernas, R. E. de Lamaestre, Ion beam-induced quantum dot synthesis in glass, In: D. Ila, J. Baglin, N. Kishimoto, P. K. Chu, (Eds), Symposium on Ion-Beam-Based Nanofabrication held at the 2007 MRS Spring Meeting, Materials Research Society, San Francisco, CA, 2007. pp.101.

[67] R. E. de Lamaestre, H. Bea, H. Bernas, J. Belloni, J. L. Marignier, Irradiation-induced Ag nanocluster nucleation in silicate glasses: Analogy with photography, Phys. Rev. B 76 (2007) 18.

[68] R. Giulian, P. Kluth, L. L. Araujo, D. J. Sprouster, A. P. Byrne, D. J. Cookson, M. C. Ridgway, Shape transformation of Pt nanoparticles induced by swift heavy-ion irradiation, Phys. Rev. B 78 (2008) 8.

[69] X. Kerbiriou, J.-M. Costantini, M. Sauzay, S. Sorieul, L. Thome, J. Jagielski, J.-J. Grob, Amorphization and dynamic annealing of hexagonal SiC upon heavy-ion irradiation: Effects on swelling and mechanical properties, Journal of Applied Physics 105 (2009) 073513.

[70] R. Kogler, A. Mucklich, L. Vines, D. Krecar, A. Kuznetsov, W. Skorupa, Study of defect engineering in the initial stage of SIMOX processing, 15th International Conference on Ion Beam Modification of Materials, Elsevier Science Bv, Taormina, Italy, 2006. pp.161.

[71] Y. Maeda, K. Umezawa, Y. Hayashi, K. Miyake, K. Ohashi, Photovoltaic properties of ion-beam synthesized beta-$FeSi_2$/n-Si heterojunctions, 46th Spring Meeting of the Japan Society of Applied Physics, Elsevier Science Sa, Chiba, Japan, 2001. pp.256.

[72] O. Picht, W. Wesch, J. Biskupek, U. Kaiser, M. A. Oliveira, A. Neves, N. A. Sobolev, Ion beam synthesis of Mn/As-based clusters in silicon, Nuclear Instruments and Methods in Physics Research Section B: Beam Interactions with Materials and Atoms 257 (2007) 90.

[73] G. Rizza, Y. Ramjauny, T. Gacoin, L. Vieille, S. Henry, Chemically synthesized gold nanoparticles embedded in a SiO_2 matrix: A model system to give insights into nucleation and growth under irradiation, Phys. Rev. B 76 (2007) 9.

[74] M. Steinert, W. Wesch, A. Undisz, M. Rettenmayr, W. C. Nunes, R. P. Borges, M. Godinho, R. M. Rubinger, M. C. Carmo, N. A. Sobolev, Ion beam synthesis of Mn/Sb clusters in silicon, J. Phys. D-Appl. Phys. 42 (2009) 6.

[75] C. W. Yuan, D. O. Yi, I. D. Sharp, S. J. Shin, C. Y. Liao, J. Guzman, J. W. A. III, E. E. Haller, D. C. Chrzan, Theory of Nanocluster Size Distributions from Ion Beam Synthesis, Physical Review Letters 102 (2009) 146101.

[76] Anonymous, User's Guide to DOE Facilities, U.S. Department of Energy, Washington, D.C.

20585, DOWER-01 74.
[77] http://train.ornl.gov/sbms/SBMSearch/subjarea/userfacility/guide.htm
[78] Basic Energy Sciences Advisory Committee, Report of the Basic Energy Sciences Advisory Committee Subpanel Review of the Electron Beam Microcharacterization Centers: Past, Present, and Future, , Department of Energy, Germantown, MD, February 2000, DOE/SC-0019.
[79] Z. Yao, M. Hernandez-Mayoral, M. L. Jenkins, M. A. Kirk, Heavy-ion irradiations of Fe and Fe-Cr model alloys Part 1: Damage evolution in thin-foils at lower doses, Philos. Mag. 88 (2008) 2851.
[80] M. Kirk, M. Li, P. Baldo, Damage Correlation Between In situ Ion Irradiation and Neutron Irradiation in Molybdenum, Microscopy & Microanalysis 2009 Meeting, Richmond, VA, 2009.

Appendix A. Attendees and Readers

Attendees

Name	Org
Todd Allen	U of WI-Madison
Robert S Averback	U of IL
Pascal Bellon	UIUC
Graham Bench	LLNL
Vasily Bulatov	LLNL
Alfredo Caro	LLNL
Daryl Chrzan	LBL/UC Berkley
Barney Doyle	SNL
Rod Ewing	U of MI
Michael Fluss	LLNL
Wayne King	LLNL
Mark Kirk	ANL
Richard Kurtz	PNNL
Bernhard Ludewigt	LBL
Stuart Maloy	LANL
Amit Misra	LANL
Mike Nastasi	LANL
Lee S. Schroeder	LBL
Magdalena Serrano De Caro	LLNL
Roger E. Stoller	ORNL
Barry Sullivan	DOE OFES
Lumin Wang	Univ of MI
Yongqiang Wang	LANL
Bill Weber	PNNL
Yanwen Zhang	PNNL

Readers

Name	Org
Matt Alinger	GE Research
Mark A. Bourke	LANL
M.Grace Burke	Bettis Lab
Larry Greenwood	PNNL
Bill Hamm	KAPL
Howard Heinisch	PNNL
Grant Logan	LBL
Michael K. Miller	ORNL
G. Robert Odette	UC Santa Barbera
John L. Sarrao	LANL
Shahram Sharafat	UCLA
Kurt E. Sickafus	LANL
Lance Snead	ORNL
Gary Was	Univ of MI
Brian Wirth	UC Berkeley
Sidney Yip	MIT
Steven Zinkle	ORNL

Appendix B. Workshop Agenda

Workshop on

Science Applications of a Triple Beam Capability for Advanced Nuclear Energy Materials

April 6-8, 2009

Building 170 Room 1091

Monday April 6, 2009

Time	Event
7:30 – 8:30	Continental breakfast, informal discussions, and check in

Time	Topic	Speaker
8:30 – 8:45 AM	Welcome	Bill Goldstein
8:45 – 9:00 AM	Purpose of workshop	Michael Fluss
9:00 – 9:15 AM	Introduction of participants	All
9:15 – 10:30 AM	Defining the scientific need: Does the US need a triple ion beam irradiation facility?	"1 slide + using provided template" presentations from all participants (see attached list of titles)
10:30 – 11:00 AM	Break	
11:00 AM – 12:30 PM	Defining the scientific need: continued	"1 slide +" presentations from all participants (see attached list of titles)
12:30 – 1:30 PM	Lunch on your own at Lab Cafeteria	
1:30 – 3:15	Round Table discussion on the specifications of such a facility	All
3:15 – 3:45 PM	Break	
3:45 – 4:45 PM	Status of theory simulation and modeling and how are they complementary	Vasily Bulatov
4:45 – 5:30 PM	Take stock and request written comments	King
6:30 – 8:00 PM	No Host dinner, @ Hilton Hotel	

Tuesday April 7, 2009

Time	Event
8:00 – 8:30	Continental breakfast, informal discussions and transit to CAMS

Time	Topic	Speaker
8:30 – 9:30 AM	Tour of CAMS	Bench
9:30 – 9:45 AM	Transit to B170	
9:45 – 10:15 AM	Relation to MTS, ATR, and HFIR	Maloy, Allen, and Stoller
10:15 – 10:30AM	Break	
10:30 – 11:00 AM	Capabilities at JANNuS, TIARA (Duet) and Kharkov	Fluss
11:00 – 11:30 AM	Capabilities at ANL, PNNL, LANL, SNL	Kirk, Zhang, Wang, Doyle
11:30 – 12:30 PM	Take stock, request written comments, and finish up	Fluss/King
12:30	Adjourn	

Writing group and workshop organizers

Time	Topic
12:30 – 1:30 PM	Lunch on your own at Lab Cafeteria
1:30 – 3:00 PM	Selected writers work on draft of workshop report
3:00 – 3:30 PM	Break
3:30 – 5:30 PM	Continue with tasks
5:30 PM	Adjourn
6:30 – 8:30 PM	No host dinner

Wednesday April 8, 2009

Time	Event
8:00 – 8:30	Continental breakfast, informal discussions

Time	Topic
8:30 – 10:00 AM	Continue with tasks
10:00 – 10:30 AM	Break
10:30 – 12:00 PM	Take stock and finish up
12:00 PM	Adjourn

Appendix C. International Triple Beam Facilities

Fundamental Materials Research Can Lower the Barriers to Advanced Nuclear Energy

The future of nuclear energy depends on advances (or lack of thereof) in materials. To make a serious impact on the future development of nuclear energy, materials R&D has to rely on accelerated experimentation that isolates and elucidates key phenomena. This is a science challenge, maybe one of the most difficult ones ever. What we are lacking in the U.S. to address this challenge are materials irradiation platforms that are fast, efficient, and allow researchers to isolate the fundamental components (unit mechanisms) of the very complex materials evolution problems faced in advanced nuclear energy systems. New ion-beam facilities are the platforms and, in a real sense, the catalysts for nuclear energy materials R&D. Coupled with materials theory and existing and planned neutron platforms, such an ion-beam facility or facilities will add critical relevance to accelerated materials research. Accelerated materials research places increased demands on materials theory. For maximum impact, accelerated materials experimental research must be fully integrated with materials theory and simulations. Multi-ion-beam facilities will help to build realistic complexity into materials models by simulating the in-growth of nuclear transmutants along with the displacement of atoms.

Accuracy and reliability of theoretical extrapolations can be significantly improved by addressing deficiencies and bottlenecks in the existing theory. There is much value in using several theoretical approaches for modeling damage accumulation in irradiated materials. Nimble, low-cost ion-beam irradiation research platforms, in tandem with efficient and accurate materials theory, can reinvigorate nuclear energy materials R&D. Multi-beam particle accelerators can (a) fill the critical research experimental gap while simulating many of the conditions of a variety of reactor environments, (b) provide training for a new generation of scientists, and (c) accelerate development of theory simulation and modeling to deal with the complexity of materials evolution in advanced nuclear energy systems.

Radiation damage accumulation takes place on a broad range of timescales. The various steps of collision–recombination–relaxation and defect migration–clustering–nucleation–growth are completed within timescales ranging from picoseconds to years. Experimentation can study the resultant static microstructure. Extension of simulation methods, particularly Monte Carlo methods for transcending the timescales of nuclear radiation damage accumulation between ion-beam and reactor neutrons, is a critical need that well-planned ion-beam experimentation can help to accelerate through careful coordination and planning.

Impact of a Triple Beam Facility on U.S. Nuclear Energy Research and Development

The interest in closing the nuclear fuel cycle results in a need to investigate much higher radiation fluence than previously envisioned for structural materials and for fuels. The paradigm of studying materials for nuclear energy applications by utilizing test reactors is in many cases problematic because of the long elapsed times to achieve the requisite neutron fluence and the limited number of facilities available for such work. Indeed, certain neutron spectra, such as those for fusion energy and fast reactors, are either nonexistent or quite limited in their availability. Moreover, there is a need for fundamental materials research in order to develop the radiation-tolerant materials requisite for a new generation of reactors and to nurture the education of future scientists.

One possibility, perhaps the only possibility, is to use multiple ion-beam irradiations in conjunction with simulation and modeling to investigate alterations in material properties at low irradiation rates (reactors) and at high rates (ion-beams). The importance of multiple ion-beam irradiations is the synergy associated with the simultaneous production of helium and hydrogen along with vacancies and interstitials from displaced atoms. Today, there are three facilities of this type: TIARA in Japan, JANNuS in France (expected to be on-line in early 2010), and a facility at Kharkov University, Kharkov, Ukraine.

With the use of a triple ion-beam platform, it is reasonable to isolate and study the fundamental mechanisms of damage accumulation, even at very high doses, in a time interval of a few hours to a few days. This leaves the issue of low-rate irradiations and long exposure times, times of many years to many decades (as in a nuclear reactor). Experiments are envisioned where specimens are preirradiated with ion-beams to conditions representing years or decades in a reactor. These specimens would then be exposed to relevant neutron spectra in a test reactor or spallation source, and the "differential" response could be studied. The conclusion is that ion-beam experimentation research can make contact with all the necessary irradiation conditions to assist in the development of rate-transcending models:

1. Low-rate, low-dose damage with multiple ion beams
2. High-rate, low-dose damage with multiple ion beams
3. High-rate, high-dose damage with multiple ion beams
4. Low-rate, high-dose damage with ion beam conditioning followed by neutrons

The User Community: National and International

As the issue of closing the fuel cycle becomes more probable, and with it the concomitant needs for high burnup and harder neutron spectra, the need for basic scientific research on the radiation response of materials (structural and fuels) becomes more important. Additionally, fusion energy researchers must ultimately also solve many of the same problems encountered with fission energy. These factors are motivating the materials community to focus on the use of ion-beams to carry out basic research in radiation-tolerant materials, high-temperature materials (both refractory alloys and ceramics), and advanced fuel concepts such as inert matrix and TRISO fuels. The IAEA has initiated a coordinated research program that weds modeling and simulation with multiple ion-beam simulations to mimic the important production of helium and hydrogen by implantation simultaneously with self-ion irradiation to produce displacements. Three facilities of this type are currently operating or are close to operation: in Japan (TIARA), Ukraine (Kharkov), and nearing completion in France (JANNuS at Saclay). Available research time for scientists outside the host institutions is limited. If the U.S. is to take advantage of multiple ion-beam research to develop advanced materials for nuclear energy, a U.S. facility will be needed.

Appendix D. Scientific Challenges Discussion

A free-wheeling discussion was held on the topic of Scientific Challenges relevant to a triple beam or multi-ion-beam facility.

R. Stoller gave his input on the history of the ORNL Triple-beam Laboratory, and provided a bibliography of relevant references from experiments carried out there. The ORNL facility was used until the late 1990s, then the general interest in supporting ion-beam irradiation diminished. The triple beam experiments supported the U.S. fast reactor and fusion materials programs, as well as fundamental defect physics. His input on the scientific needs included comments on the kind of science that can be done today.

Discussion: Mechanisms of synergistic effects, effects on properties of new materials for fusion, IFMIF, and TMS are mentioned, as well as spallation sources and advanced reactors. Would it be possible to help down-select materials? Will the theory, modeling/simulation help? What is the BES perception? A briefing will be prepared on the outcome of this workshop.

M. Nastasi provided his input on scientific needs. Ionization effects and ion/neutron interactions are part of the list. He mentions the possibility of co-location of triple beam with a light source, and TEM. What would be the triple beam accomplishments?

Discussion Modeling should be leading the triple beam project. Would it be possible to offer a "package" that includes triple beam irradiations, in-situ diagnostic capabilities, and in-situ modeling? The discussion follows on the number of local and international users, public reach, patents, etc.

How do we look at the triple beam project from the "fundamental understanding" BES perspective? B. Weber mentions modeling of different phenomena, like nucleation rate, bubble formation, as a function of dose rate.

Y. Zhang mentions the possibility of measuring fundamental properties, and the fact that electronic stopping power calculations for some compounds are different from experimental findings by a factor of 2 to 3.

B. Weber mentions effects of rate on waste forms, SNF, and situations where only empirical models exist.

Discussion The possibility is open to other materials: fuels, oxides, nitrides, carbides, inert matrix, ceramic composites, ZrC, SiC, materials used in HTGRs and waste-forms, where fundamental studies are needed.

R. Ewing mentions the field of first-principle modeling of actinides. The science area is just waiting to be investigated and will reveal a lot of surprises. Issues are raised relative to producing samples, fabricating containments, etc. Fundamental science will be everlasting, while decisions on the specific nuclear program can change. A triple beam facility will help answer fundamental question that will enable intelligent decisions.

Discussion Is it possible to design a project that attracts the scientific community and generates an educated workforce?

B. Averback gives his input on scientific needs, emphasizing creativity, diversity, original good ideas. He says that 99% of the scientific population does not have access to major home facilities. The proposals are written without them. He says in-situ TEM and all kinds of post-analysis stages are greatly needed. He mentions in-situ training stages as a major advantage of such a triple beam facility. He proposes a National Ion Beam User Facility encompassing a large number of in-situ and post-irradiation characterization tools.

Issues are raised relative to user facilities made available easily to the public without cumbersome bureaucratic procedures.

G. Bench mentions that the LLNL-CAMS ion-beam facility is a good example of an educational center that received thousands of visitors in 10 years, produced hundreds of Masters and Ph.D. theses, and hosted in the past 10 years faculty members, students, for periods of weeks to months, with funding provided by UC. Emphasis is made on the general open door policy.

M. Nastasi, and ***B. Weber*** mention facilities "outside the fence" with computer network systems, student access, etc.

R. Kurtz presents the view of the scientific needs from the perspective of the fusion community. He mentions as an example the effect of solid transmutants on fusion materials, compatibility of materials with coolants, behavior of ODS steels that show excellent thermal stability. He suggests the possibility of doing triple beam experiments of "materials under load." Robust modeling is needed to interpret these results. Experiments must be put in contrast to the existing modeling. Advances are made possible by utilizing the limited experimental volume much more efficiently. In IFMIF, MTS volumes of high flux space are small and there is the need of obtaining fusion-relevant EOL doses. Issues relative to surface versus bulk irradiations are raised and whether or not 10 grains is a limit. ODS steels show extremely small grain sizes. Would a couple of grains be enough? Investigations are ongoing on He trapping in ODS steels, and He migration to grain boundaries (He levels required of 1000 appm, and doses of 200 dpa).

B. Doyle mentions the potential tritium build-up problem in neutron-damaged FW diverter materials in ITER, and experiments at SNL and General Atomics using combined mono-beam exposures of W to 28 MeV Si (at SNL) to simulate multiple dpa levels of fusion neutron damage and ^{2}D plasma exposures (at GA) to simulate FW conditions at the ITER diverter. Initial experiments have already been published and have shown that the additional tritium buildup in the ITER diverter due to neutron-induced displacement damage will be small compared to the allowed tritium inventory at ITER. On the other hand, blistering was observed too, and this may be a problem as regards plasma impurity effects.

M. Fluss envisages the possibility of designing clever experiments that would isolate components of the scientific problem. Fundamental studies coupled with enhanced experiments are available today and were not there before. Research has to be smarter, cautious. The decision on which material is going to be taken to the neutron facility must be made with solid background information. Triple beam offers the advantage of fast procedures, no cooling, and small samples. Results of these investigations will impact the nature of the facilities that are coming. ***R. Stoller*** mentions that experiments with neutrons are required to obtain data on bulk mechanical property specimens in order to qualify the materials. The discussion proceeds on the cost of expensive diagnostics and exploration of radiation damage effects on materials with a wide range of tools.

B. Doyle gives his input on scientific needs underlying the fact that this is a fruitful area for this country to be moving on. He mentions that current ion sources produce the same rate of appm He as in reactors. He mentions the design of a new building at SNL (to be completed a year from now) and ongoing LDRDs and MFE programs, and projects proposed to BES in his lab that would utilize this proposed new facility if it were available now.

D. Chrzan gives his input on scientific need from another perspective. High-dose effects are under investigation in the semiconductor community. His perspective is that of "theory and experiments" and the possibility of a triple beam facility opening up

to the silicon-user scientist. He mentions modeling for nucleation and growth Yuan (2009), growth of binary nanocrystals, junctions, and the theory that describes different regimes and the competition of coarsening versus damage processes.

The triple beam project could open to nonexperts in the radiation effects field.

M. Fluss mentions the possibility of controlling stochiometry by ion-beam synthesis. The fact is that there is little or minimum control on the process in the way of producing ODS steels with nanodispersoids by ball milling and heat treatments.

S. Maloy input underlines the need of developing materials to stand high doses, push the fuel burnup limit beyond 40%, and reach doses of 200–450 dpa at temperatures in the range of 400–600 °C. He mentions the possibility of the triple beam adding information to supplement the materials side research done within AFCI on fundamental aspects of RIS, void swelling, fuel/clad interaction, and ion-irradiation of minor actinides. From this perspective, 3- or 4-beam irradiation of fuels and coatings is useful, investigating dpa + fission track damage, fission gas accumulation, etc.

T. Allen input on the scientific need emphasizes the ability of modeling to close different levels better than in the past. He raised the question: Can we get a better understanding of more complex alloys? How complex a system can be analyzed today—can we push forward the scientific frontier? The question is raised on the "middle ground" between fundamental science and the technological perspective:

Will a triple beam capability facilitate the bridging?

Lumin Wang mentions the progress in simulation of radiation damage in nuclear waste forms, and the progress in in-situ creep testing and high temperature stage available at the University of Michigan. A reference is made to the work published by J. Lian, L. M. Wang, K. Sun, and R. C. Ewing, in the Microscopy Research and Techniques Journal in 2009, and on effects of ionizing radiation in ceramics.

B. Weber underlines the need of ion-beam data to quantitatively model materials and extrapolate to a neutron environment.

M. Kirk mentions that the ion-beam/TEM facility at ANL will be down in 5 years. He presents slides that emphasize thin foils research. He suggests the study of simple systems and experiments that can be compared with neutron irradiations.

P. Bellon mentions the effort at Saclay. U.S. proposals to access the facilities are mentioned. The operation is very costly (€7000 per day; €2000 per day depending on the complexity).

Appendix E. Scientific Challenge Slides

Scientific challenges	Triple beam research
▪ Effect of transmutation gasses on high-dose void swelling response (cladding and duct) ▪ Microstructural trapping of transmutation gasses ▪ Hydriding under irradiation ▪ Fission gas nucleation and growth	▪ He, H and damaging species in metals ▪ Fission gas and damaging species

Potential scientific impact	Impact on nuclear energy systems
▪ Extended dose cladding and duct materials ▪ Use of high nickel alloys in radiation fields ▪ Actinide bearing fuel science	▪ Minimize nuclear waste and improve economic impact through higher burnup ▪ Improved higher temp operation ▪ Studies in parallel with reactor studies

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Scientific challenges	Triple beam research
▪ Detailed control of ion beam synthesis of nanostructures ▪ Controlled transmutation doping of nanostructures	▪ Ion Beam Synthesis of Nanostructures: Developing detailed models/experiments that enable the controlled synthesis of nanostructures.

Potential scientific impact	Impact on nuclear energy systems
▪ Predictive models for the structures that develop at high dose implants	▪ Modeling approach will lend insight into radiation damage processes for a broad range of rates and temperatures.

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Scientific challenges

- A triple-beam facility could be used to investigate specific scientific questions such as the synergistic effects of high displacement damage coupled with co-deposition of transmutation products.
  - Triple-beam research would not eliminate the need for a fusion relevant neutron source.
  - A neutron source is essential for producing bulk property information.

Triple beam research

- Explore synergistic effects of simultaneous self-ion displacement damage with He and/or H injection.
- Investigate solid transmutants on microstructural evolution (e.g. Mg in SiC
- Phase stability of Y-Ti-O nanoclusters in nanocomposited ferritic alloys.
- Microstructural evolution of stressed specimens under irradiation.

Potential scientific impact

- Improved understanding of the fundamental mechanisms of specific radiation-induced damage phenomena.
- Advancement of physics-based models of complex material behavior under irradiation.

Impact on nuclear energy systems

- Enhance basic scientific understanding to more efficiently utilize the limited volume of a fusion neutron source.

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Scientific challenges

- Scientific basis for radiation tolerant materials for nuclear energy systems
- Synergistic effects of radiation damage and nuclear transmutants
- Realistic modeling of radiation damage accumulation over decades at the rates of nuclear energy systems
- Evolution of microstructures in complex actinide systems and their physical properties
- Fundamental understanding of similarities and differences between ion-solid interactions and neutron-solid interactions

Potential scientific impact

List the scientific accomplishments by which the success of the facility will be measured:

- The same as any other user facilities - the number of national and international users, publications, presentations, patents, easy access by foreign nationals, etc.

Important strategies for realizing this impact

- Co-location with other characterization facilities: TEM; light source; neutron source; high energy protons (radiography, irradiation, etc.).
- Identification of which material properties can be simulated with a triple ion beam and which can not

Triple beam research

Accelerated simulations of materials in extreme neutron irradiatio environments.

- Study of the combined effects of target damaging through nucle and electronic energy deposition and ion implantation effects (simulation of helium, hydrogen and fission product production, and other transmutation reactions)) under a wide range of temperature and environmental conditions.
- Combined irradiation with ion beam analysis (characterization).

Impact on nuclear energy systems

How do you envision success contributing to the development of materials for nuclear energy?

How will this facility complement the use of various existing and planned neutron sources?

- The purpose of these facilities will be to systematically explore the role the various components that represent a neutron-solid interaction to determine elementary chemical–physical mechanisms involved in the evolution of the microstructure, the surface reactivity or the physical an mechanical properties of materials under neutron irradiation.
- The information gained from these experiments will be used to provide:
  - Validation of modeling, theory, and simulation predictions
  - Allow for the prescreening of candidate materials under extreme irradi conditions prior to testing in more traditional neutron environments.
- Can easily implement in-situ diagnostics and timely sample access for p irradiation characterization due to no or low activation of the targets by irradiation.

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Scientific challenges	Triple beam research
▪ Scientific basis for radiation tolerant materials for nuclear waste management ▪ Synergistic effects of electronic and nuclear stopping in ceramics ▪ Evolution of radiation damage in complex ceramic materials and their physical and chemical properties	▪ Better prediction of radiation damage in nuclear waste forms due to the decay of radioactive elements that generate multiple energetic charged particles simultaneously

Potential scientific impact	Impact on nuclear energy systems
▪ Better understanding the complex radiation damage processes under multiple radiation source ▪ Provide more realistic data for advanced models	▪ Better scientific understanding leading to better models for prediction of long term behavior ▪ This facility complement the use of various existing and planned neutron sources (none radioactive samples)

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Scientific challenges	Triple beam research
▪ Mechanisms for radiation tolerance in nuclear ceramics and composites (fuels, composite fuels, structural composites, waste forms) ▪ Predictive models for microstructure evolution and performance in nuclear ceramics and composites ▪ Validated models of radiation damage and gas accumulation on microstructure	▪ Simultaneous irradiation with self ions to limit chemistry changes and maintain stoichiometry (M/O ratio) ▪ Simultaneous irradiation with gas atoms to investigate void and bubble formation ▪ In situ, periodic ion-beam analysis of damage accumulation ▪ In situ TEM of dual beam irradiation damage

Potential scientific impact	Impact on nuclear energy systems
▪ High impact publications ▪ Acceptance of validated models ▪ Training next generation of nuclear material scientists	▪ Validated, predictive models from well-controlled experiments that can be used for the complex environments of nuclear energy systems ▪ The understanding and predictive models will be further validated and refined used neutron sources

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Scientific challenges	Triple beam research
▪ Role of coupled electronic and atomic dynamics on the evolution of ion-beam damage in nonmetallic systems, and impact on predictive models at realistic rates in nuclear environments ▪ Theory & models of electronic stopping power in compounds are inaccurate ▪ Effects of transmutants on properties	▪ Experimental & computational methods to study & model effects of electronic excitations on defect production & migration, microstructural evolution, nonequilibrium thermodynamics, & phase transformations ▪ Develop accurate theory/model of electronic stopping for compounds

Potential scientific impact	Impact on nuclear energy systems
▪ Comprehensive understanding & models of radiation effects in nonmetals ▪ Simulation methods for coupling of electronic & atomic dynamics	▪ Better predictive understanding of nuclear waste forms and spent fuel ▪ Advanced waste forms ▪ Fuel and reactor performance codes that are based on physical models and not empirical correlations

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Appendix F. Correlation of Workshop Scientific Challenges

Workshop participants described numerous scientific challenges (see Appendix C). The organizers have attempted to bin these many challenges to five grand challenges. The following table shows how the organizers have binned the scientific challenges presented by the participants.

Challenge 1

Microstructural and synergistic effects of high displacement damage coupled with implantation of transmutation products
Effect of transmutation gasses on high dose void swelling response (cladding and duct)
Microstructural trapping of transmutation gasses
Fission gas nucleation and growth
synergistic effects of high displacement damage coupled with codeposition of transmutation products
Scientific basis for radiation tolerant materials for nuclear energy Systems
Synergistic effects of radiation damage and nuclear transmutants

Challenge 2

Evolution of microstructure, physical and chemical properties in complex actinide fuels and nuclear waste management materials
Hydriding under irradiation
Evolution of microstructures in complex actinide systems and their physical properties
Evolution of radiation damage in complex ceramic materials and their physical and chemical properties
Effects of transmutants on properties

Challenge 3

Realistic modeling of radiation damage accumulation over decades as in a nuclear energy system
Realistic modeling of radiation damage accumulation over decades at the rates of nuclear energy systems
Fundamental understanding of similarities and differences between ion-solid interactions and neutron-solid interactions
Mechanisms for radiation tolerance in nuclear ceramics and composites (fuels, composite fuels, structural composites, waste forms)
Predictive models for microstructure evolution and performance in nuclear ceramics and composites
Validated models of radiation damage and gas accumulation on microstructure
Theory & models of electronic stopping power in compounds are inaccurate

Challenge 4

Detailed understanding of coupled electronic and atomic dynamics on the evolution of ion-beam damage including the combined effects of electronic and nuclear stopping
Scientific basis for radiation tolerant materials for nuclear waste management
Synergistic effects of electronic and nuclear stopping in ceramics
Role of coupled electronic and atomic dynamics on the evolution of ion-beam damage in nonmetallic systems, and impact on predictive models at

Challenge 5

Detailed control of ion beam synthesis and transmutation doping of nanostructures
Detailed control of ion beam synthesis of nanostructures
Controlled transmutation doping of nanostructures

Appendix G. Alignment with Energy Challenges Described in the BESAC Grand Challenges and the Basic Research Needs Series

Impact on Understanding Matter Far From Equilibrium

The envisioned high-energy (MeV) triple ion-beam irradiation facility is well-correlated with the Basic Energy Sciences Advisory Committee (BESAC) grand challenge: "How do we characterize and control matter away – especially very far away – from equilibrium?" [45] Energetic ions can be used to produce well-controlled defect (far from equilibrium) structures in materials that provide insight into the damage processes in advanced nuclear energy systems (ANES). This requires us to link concepts over a broad range of length scales from the atomic to the macroscopic and timescales from femtoseconds (the time it takes to create a single damage cascade) to hours and years (the time it takes for the defect structures to evolve and effect macroscopic properties).

Bridging of these length and time scales will require development of a quantitative understanding of nonequilibrium dynamics, processes, and configurations in terms of a tractable number of variables, i.e., an understanding of the unit mechanisms that govern the behavior. We will need to answer questions such as those posed by BESAC, "What are the general rules that apply to microscopic relaxation time scales that are very long? Can we comprehend how systems search free-energy landscapes?" Success will only be achieved through a close coupling of well-controlled experiments with forefront theory, simulation, and modeling.

With experimentally validated models founded upon a firm understanding of the unit mechanisms, we can begin to consider how we might apply this knowledge to the development of materials that are irradiation-damage tolerant, or even irradiation-damage immune, by stabilizing matter in nonequilibrium states. With detailed knowledge of mechanisms and kinetics, perhaps we could even consider the possibility of developing materials that are self-repairing to the effects of irradiation.

Alignment with the Basic Research Needs Workshop Reports

A high-energy (MeV) triple ion-beam irradiation facility is expected to impact science related to the Basic Research Needs Workshop Reports on Materials under Extreme Environments[46] and Advanced Nuclear Energy Systems [1]. For both of these reports, the issues of bridging time and length scales, the potential for damage-tolerant or damage-immune materials, and the potential for self-healing materials, are intersected by the science that could be carried out at such a facility.

Workshop participants particularly pointed out the potential importance of a high-energy (MeV) triple ion-beam irradiation facility in enabling science related to irradiation, transmutation, and radiolysis effects in nonmetals in general, and actinide fuels and waste forms in particular. While this was seen as perhaps the biggest growth area, it was recognized that this area has relatively few active researchers. Further, simulation and modeling is not as advanced for these materials as in the case of metals.

Because of the unique capability to reach irradiation doses that are not obtainable in neutron sources, this facility and associated theory, simulation, and modeling will play a key role in establishing knowledge of the absolute physical limits of materials behavior in extreme energetic flux environments and the damage evolution mechanisms that lead to materials degradation and failure. The term used most often in the BRN workshop reports is "accelerated radiation effects test methods." It will also play a key role in providing data required for validating length and time scale bridging models and simulations.

The workshop participants, as in the workshop on materials in extreme environments, cited the potential for nonequilibrium synthesis and processing with energetic particle and photon beams (see discussion above).

The scientific challenges posed by advancing the technologies of nuclear energy are easy to identify yet difficult to master. Looking into the future, nuclear energy systems will demand new materials—materials operating at higher temperatures, for longer periods of time, and in neutron spectra that result in a more complex mixture of radiation damage components. This is particularly the case with nuclear reaction transmutants of hydrogen and helium, along with vacancy and interstitial point and extended defects. The technological goal of closing the fuel cycle raises materials issues not previously faced by the nuclear energy industry, and which require the best scientific minds to find the appropriate answers. At the highest level, there are three overarching materials issues:

1. Controlling the consequences of radiation damage accumulation in structural materials through fundamentally-based materials design.

2. Controlling the evolution of nuclear fuels through a basic understanding of the evolution of complex mixtures of actinides and the fission products in materials systems that combine the desired properties of containment and thermal conductivity.

3. Controlling the effects of self-radiation damage and transmutations on the aging and evolution of nuclear waste forms

This workshop has focused on providing a scientifically robust path forward for dealing with the vexing issues of basic materials research for nuclear energy applications through the application of multiple ion-beam research. First is that the timescales of the phenomena that are taking place in the neutron environment are often on a scale of decades and neutron materials research facilities cannot be expected to accelerate that rate by more than a factor of two to five. In addition, it is often the case that the specific neutron spectra required to simulate a particular radiation condition is not available. For example, this is often the case for the materials research on fusion energy materials. A triple ion-beam facility provides the materials community with a unique research platform that meets several of the goals laid out in this report[1], including Materials Under Extreme Conditions, Chemistry Under Extreme Conditions, Advanced Actinide Fuels, Advanced Waste Forms , and Predictive Modeling and Simulation.

Appendix H. Discussion of Theory, Simulation, and Modeling

Discussions and comments with respect to the integral role that theory, simulation, and modeling will play in a triple ion-beam facility follow:

V. Bulatov introduces the topic of theory, simulation, and modeling (TSM) and accelerated materials testing (AMT), and the possibility of going "top-down" in the modeling of radiation damage and the use of rate-theory. The question is raised whether or not different dose-rates will give rise to different microstructures. A theory on charge state of insulating materials is not available. Large, intense radiation environments depend on modeling. Model-based programs are needed.

D. Chrzan raises the question on the role of the center. Can it expand beyond nuclear materials applications? Address the physics of materials damage, He, H ions, electronic excitations (semiconductors), problems that are relevant a long time after the cascade develops and have a significant effect on how the cascade takes place. Time-dependent ab-initio calculations are mentioned. Should we look into charge effects on local mobilities? How does this affect migrations energies (SiC)? Understand the dependence on the lifetime of these charged states. A too-narrow focus should be avoided.

R. Ewing mentions decay damage in nuclear waste forms. Ion beam science could contribute and has contributed to this field. A model is sought that can describe what happens after the cascade takes place; produce the information on how the microstructure will evolve after that.

A. Misra asks whether a methodology could be developed to model ODS. What kind of modeling could be done? ***A. Caro*** says that the problem is difficult. It is difficult to simulate oxide-metals' interphases. He suggests working on model systems that are much simpler. He mentions the problem of phonon, heat transport, and the fact that scattering of electrons with ions will affect the lifetime and have an effect on the outcome of the cascade.

P. Bellon says that simulations over different length scales and rates are important. Simulations are needed to reveal important features, and to design experiments. These features come so strong in the model, are so robust, that they will eventually show in a well-designed experiment. TSM is great to discover mechanisms. Such modeling tools offer the possibility to take a closer look at a feature, then look at the experiment and see if what happens in the model occurs experimentally.

Discussion: Concerning ODS, the question is raised whether or not it would be possible that modeling could constitute a guide to design relevant experiments. Comment: It will be nice to design an experiment within the lifetime of a graduate student.

Could it be possible to design triple beam experiments that match neutron irradiations?

T. Allen mentions the need of coupling experiment and modeling. The existence of a "no man's land" is mentioned, i.e., a "middle ground" region where nobody is working. ***R. Stoller*** mentions that controversies on the comparison of ion and neutron irradiations, which arose in the 1980s, are not yet resolved. Could we do that today? The discussion proceeds on dpa-rate effects and He effects on complex materials.

Today, QA and licensing require tests in a neutron reactor. Future neutron sources like IFMIF and MTS are mentioned. There is a need to acquire significant amounts of data to underpin models. The need of a similar neutron spectrum is raised. ***B. Averback*** raised the question on an ion PKA spectrum: How close is that to fusion? Neutron sources are also

simulations to some extent. Could we tailor the ion-beam so that it matches the corresponding PKA spectrum?

Discussion: The argument follows on the size of the samples. Samples have to be thick. How much? ~10 grains? This is empirical information. Why 10 grains? Why not 8? Is it possible to extract valuable information from something smaller than 10 grains? Can we deal with "things" that approach the bulk behavior? DEMO is on the roadmap, but component tests are in between. R. Kurtz says that there are big opportunities for modeling.

Discussion: Can we do experiments in a triple beam facility that are significant and will take a much longer time in a neutron environment? Can we get some answers with ion-beam irradiations that will affect, to a first order, the designs for DEMO or other systems? The discussion proceeds on understanding surface effects, coatings interfaces, refractory barriers, etc.

Discussion: This raises the question on target chamber configuration and the way samples are loaded, the accurate acquisition of temperature, and control of the irradiation parameter, to define benchmarks against which models can be tested.

Appendix I. Discussion on Multiple Ion-Beam Facility Specifications

A roundtable discussion was held on the topic of specifications for a multiple ion-beam user facility. Some of the comments are described below.

Rod Ewing gives his input on the scientific need for a triple ion-beam facility. As an example, he comments on studies of the morphology of individual tracks in GdZr, Gd Ti. These experiments are performed with heavy ions (Xe and Au). Some of these heavy ion experiments are performed at GSI (Darmstad, Germany).

Discussion: The question is raised on whether or not we have similar or more performing facilities here in the U.S. and on the science needed to understand the track formation mechanisms and radiation damage of the charged particles in relevant materials.

Michael Fluss raises the question on whether or not we understand "cascade dynamics." The collective answer is "yes and no." Yes, we know a lot more on cascade dynamics today, and no, we are not yet able to engineer a material for radiation survival. A discussion follows on whether or not a quantitative prediction is important. How do we handle phonon relaxation of the cascade? At present, we do not really include the electronic structure in our simulations. A discussion follows on the relative importance for metals, semiconductors, and ionic materials.

B. Averback noted that results are almost right and that what is important is what happens after the cascade. ***R. Stoller*** agrees on the importance of looking at the results of the cascade evolution beyond the initial ~10 to 20 ps of peak energy dissipation.

M. Nastasi comments on the evolution of the morphology of grains during the irradiation experiment. The possibility of performing in-situ experiments and in-situ microscopy is discussed and may be assigned a high priority.

Discussion: A high-resolution microscope and in-situ imaging at the atomic level are capabilities that would allow studies of the evolution of ODS nano-dispersoids, different mechanisms having an effect on CuNb interphases, etc.

Discussion: On-line diagnostics is proposed. The former Positron Annihilation studies performed at LLNL are mentioned. The possibility of performing "ultra-fast" spectroscopy and irradiation with clusters are envisaged.

The triple ion-beam should provide capabilities that "complement" those already available. ***W. King*** raises the question: Which techniques would be at the top of the list?

The number of subscriptions to JANNuS has already limited its time-availability. ***P. Bellon*** says that it is hard to say how this will be, and that one should wait a couple of years to see how much JANNuS will be used. The intention is to make it an international facility and increase the time available to external users.

Discussion: The question is raised on ANL and ORNL facilities and the user demand picking up again. Science aspects are crucial. Also, the possibility of an experiment that demonstrates the value of a triple beam facility is mentioned.

B. Weber introduces the luminescence capabilities at PNNL. He mentions depth profiling of silicon, coimplanting of He, and studies at high temperature and high dose.

M. Fluss mentions the possibility of performing isochronal annealing studies. Would it be possible to transfer the specimen after ion-irradiation to

an isochronal specimen analyzer? Would this be of importance in semiconductors (evolution at low temperature)? What about metals?

Discussion: The question leads to the discussion of standard chambers built for a special purpose, and other systems with several sample holders. A. Misra suggests in-situ TEM, and the study of mechanical properties on TEM foils.

R. Kurtz gives the "fusion" perspective. In fusion, "bulk" properties are needed (~0.25-mm-thick samples). Studies are linked to effects of stress on the microstructural evolution and propagation of plastic flow from grain to grain. High-temperature high-dose, He, H effects, and information about the evolution with temperature are crucial. Materials like steels, refractory metals, SiC/SiC composites. Experiments that make use of heavy ions, solid transmutants (Mg, Al), and the possibility of simulating a fusion PKA spectrum are mentioned. Capabilities like in-situ nanoindentation and TEM analysis to get mechanical properties, study segregation effects, grain boundaries, etc. The discussion proceeds on pillars in single crystals and micro-compression experiments. The possibility of in-situ microdiffraction experiments is mentioned.

Discussion: Dose-rate effects and the simulation of the fission together with the consequences of mass transport are problems that are valuable in fuel studies. Developing a surrogate actinide material that could be used to look to radiation effects and simulate high burnup fuels is suggested. The question is raised: Is it possible to do these kinds of studies with ion beams?

The possibility of preparing micron-sized columns with focused-ion beam milling and studying their time-dependent deformation is very attractive, but costly. ***T. Allen*** mentions the possibility of partnering with other institutions with FIB capabilities. Could the sample preparation and post-irradiation experiments be conducted at the home institution? What happens with actinide materials? Handling is needed in place to get them mounted and retrieved. Could that be envisaged?

Discussion: ANL has a focused ion-beam (FIB) and scanning electron microscope (SEM) (for sample milling, etching, analysis at high resolution) dedicated for outside use. The connection between National Labs and the universities is discussed. Will the production of micropillars saturate the use of the FIB? Will the FIB use more time than the triple ion-beam experiment itself?

Discussion: The main problem is the need of having young "new" scientists carry on with radiation studies. How do we generate an attractive research platform that attracts scientists from universities? Would it be possible to start slowly and build on the achievements?

Discussion: The need for an operator for a FIB, the problem of having people at the university that use the FIB properly and prepare samples, suggests that just handling the training is a major problem (and could be a major benefit) of such a project. A consequence is that such a facility needs adequate "staff," otherwise it is useless.

B. Averback seeks to introduce a broader concept of the triple beam facility. It should be proposed as an important Materials Science–"Radiation Studies" project. It should not be focused on addressing engineering problems relative to major nuclear programs, but further the radiation damage science field. Research does take a long time. Universities must be included. The perspective of long-term projects is desirable.

Discussion: The option of seeking funds based on engineered oriented interests while addressing fundamental materials science problems can lead to an attractive proposal. Would an Ion Beam Mate-

rials Science User's Center be of interest to BES? Would this facility have sample preparation and in-situ diagnostics? Would this community (the TEM community) consider an upgrade of the existing facilities and the coexistence of a triple beam facility elsewhere? The discussion proceeds on whether it is better to have everything in one place or not. Costs for the center equipment and staff (infrastructure cost, maintenance, keeping it operating) are much higher in the first case.

R. Ewing comments on fuels and nuclear technology and the fluctuations in the nuclear fate. The triple beam opens the possibility of thinking broadly and adjusting to the renaissance of ion beam–nanoscience centers. The discussion proceeds on the possibility of preparing an integrated package to provide the U.S. with a capability that existed previously and disappeared, and that today could bring so much exciting science.

Discussion: Research programs should be there long enough to sustain student Ph.D. theses. Could we allow continuous operation (no shutdown), avoiding large interruptions, allowing for no cool-down time of the sample? The possibility of preparing proposals that connect the facility with universities, helping them do the PIE experiments, is mentioned, together with the fact that the facility at ANL might be closed in 5 years, and that groups are looking for a second facility to perform their experiments. The question is raised on what are the experiments that would lead the priority list.