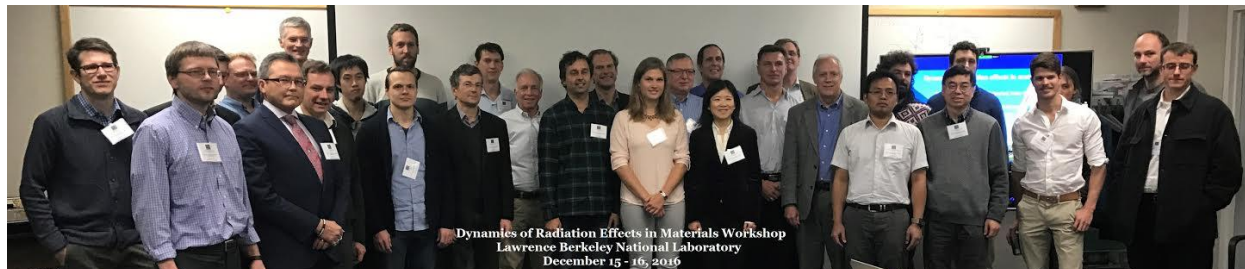


Workshop Report: Dynamics of Radiation Effects in Materials

Thomas Schenkel and Peter Seidl

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We held a workshop on the Dynamics of Radiation Effects in Materials at Berkeley Lab, Dec. 15-16, 2016. The workshop charge was to assess and discuss opportunities to access the dynamics of radiation effects. The workshop was attended by over 40 scientists from US universities, national laboratories and from institutions overseas.



The study of radiation effects in materials has a long and successful history, supporting and enabling a broad series of advances of critical importance to the mission of DOE. These include fundamental science and applications in the development of materials for current and future fusion devices, nuclear reactors and instrumentation for high performance accelerators. The field of radiation effects in materials is one example of the synergistic interplay of basic theoretical studies, modeling, simulations and experiments in selected application areas. Arguably the most impactful and ambitious application area for materials in high radiation environments is future fusion reactors. The significant materials challenges for the realization of viable fusion reactors were recently reviewed in the DOE Fusion Energy Sciences workshop report on [Plasma Materials Interactions](https://science.energy.gov/fes/community-resources/workshop-reports/) (<https://science.energy.gov/fes/community-resources/workshop-reports/>). This report identified accessing the dynamics of radiation effects in (fusion) materials as one exciting emerging opportunity that “could transform our understanding of ion-induced damage” (P. 116).

The goal of our workshop was to follow up on this observation and to connect known challenges in fusion materials science (including neutron damage, tungsten fuzz, helium bubbles, hydrogen retention and the disruptive effects of edge localized modes in Tokamaks) and broader application areas (including nuclear energy, high intensity accelerators and radiation effects on electronics) with the emerging opportunity of accessing the dynamics of these radiation effects. Here, significant advances in our fundamental understanding of radiation effects can be anticipated in the next period due the rapid emergence of a series of pump and probe tools. These will soon enable access to multi-scale dynamics from femto-seconds to seconds, and from sub-nanometers to microns and millimeters. Such experimental advances promise to deliver data that can benchmark widely used simulation codes for the first time, leading to greatly enhanced predictive power of simulations. The impact potential of these advances is enormous and matches the magnitude of the grand challenge of viable fusion reactors, as well as the importance of critically needed advanced materials for nuclear energy, high performance accelerators and radiation hard electronics.

Thus the guiding questions of our workshop were:

- What experimental results on dynamics of radiation effects can have significant impact
 - to benchmark simulations and enhance their predictive power?
 - to guide materials discovery, e. g. for enhanced radiation resistance?
- What experiments are possible now, soon and in 5 years? What developments are needed?

To address these, our workshop was organized in a series of sessions with talks covering

- modeling and simulation of radiation effects
- radiation materials science for fusion, nuclear and other applications
- experimental approaches to access dynamics of radiation effects

The opening talk by Steve Zinkle described the problem space of “Dynamic Defect Production and Recombination Phenomena in Materials”. While principal trends in many materials are known, there exists a gap of many orders of magnitude between the time scale of widely used molecular dynamics simulations and experiments. As examples, measurements that could quantify (time dependent) atomic interaction potentials and multi-scale tracking of (temperature dependent) correlated recombination effects promise to greatly enhance the predictive power of the simulations. This can enable more rapid design and discovery of materials with properties tailored to specific applications (e. g. divertor materials).

The presentations and discussions highlighted progress in advanced experimental and theory/simulation studies of radiation effects in materials. As one example, ion scattering studies promise to quantify fundamental input parameters for simulations such as atomic interaction potentials for hydrogen on tungsten. Advances in radiation effects studies via the control of irradiation and annealing temperatures and ex situ structural analysis can access the kinetics of radiation effects in nuclear materials. These experiments could be complemented with pump-probe experiments (e. g. with pulsed ion beams and a future hard x-ray FEL probe) leading to significant advances in our understanding of multi-scale materials dynamics. Dynamic effects can currently be tracked indirectly through sequences of irradiations followed by ex situ analysis of materials. Significant progress has been made in integrated studies of high resolution transmission electron microscopy of irradiated materials with molecular dynamics simulations that allow tracking of microscopic irradiation mechanisms including synergies of electronic and nuclear energy loss processes in nuclear ceramics. Combinations of ion irradiation with in situ high resolution electron or ion microscopy and mechanical testing enable unprecedented access to the dynamics of individual defect and dislocation complexes on a time scale of fractions of a second, in part enabled by the unique capabilities of helium ion microscopes for in situ irradiation and high resolution imaging. Further, the development of direct electron detectors is currently revolutionizing electron microscopy, enabling scanning electron nano-beam diffraction with unprecedented spatial resolution and sensitivity e. g. for strain mapping in irradiated alloys and around helium bubbles.

The next generation linear plasma device, the Material Plasma Exposure Experiment (MPEX at ORNL) will greatly enhance our understanding of plasma and irradiation effects on fusion materials mimicking realistic reactor conditions, where synergies of plasma exposure and neutron damage can affect materials stability and hydrogen retention.

Following these examples of advanced studies on a time scale of (many) seconds and with ex situ probes, a series of talks highlighted advances of experiments on a millisecond time scale. Defect dynamics on a millisecond time scale has become accessible with millisecond ion beam pulses combined with ex situ structural probes, and in single ion irradiations integrated with a transmission electron microscope. Recent advances now enable direct in situ detection of single ion strikes for a series of ions and substrates, which enables tracking of defect complexes with a spatial resolution of a few nanometers and a time resolution of about 10 milliseconds in important materials. Irradiations with millisecond ion pulses have revealed surprisingly long, millisecond scale defect lifetimes in silicon and SiC and 100 nm scale defect diffusion lengths. These experimental advances can now inform advanced modeling tools.

While these advances on a one to ten millisecond time scale are remarkable, they still leave us with a gap of about six orders of magnitude to the 1 ns time scale of molecular dynamics simulations (possibly extended to 1 micro second in recent developments) and with a still larger gap to the femto-second to pico-second time scale of collision cascades. Here, the emergence of novel pump-probe techniques promises to close this gap. Advances in the development of short ion pulses now enable the use of 2 to 100 ns ion beam pulses for material studies (Table 1). Ion pulses can act as the “pump” that

excites defect dynamics in a material and is followed by an (ultra-) fast probe pulse that tracks the ensuing structural dynamics. We heard talks on a series of pulsed ion beam approaches, from random single ion strikes that can be imaged on a millisecond time scale, to very high peak power ion pulses from diode type accelerators with 40 to 100 ns pulse lengths. With fast kickers sub-20 ns ion pulses can be formed at electrostatic ion accelerators and while the number of ions per pulse is relatively small (or order 10^4 ions/pulse/mm²) these short pulses enable studies of dose rate effects on electronic devices. Induction accelerators, such as NDCX-II at LBNL, now deliver about 2 ns ion pulses with peak currents of ~ 1 A/mm². Laser-plasma driven acceleration of ions provides a few pico-second ion pulses, but ballistic de-bunching spreads the pulse length to a few ns unless re-bunching techniques are applied. Intense ion pulses already provide access to defect dynamics today on a nanosecond time scale but with limited diagnostics. An exciting next step is the pairing of advanced probes with these novel pump-techniques.

Table 1: Examples of ion beam pump technologies

	Electrostatic ion accelerators	Pulsed power diodes	Induction accelerator	Laser plasma acceleration
Ion pulse length	~ 15 ns to ~ 1 ms and cw	40 to 100 ns	2 to 20 ns	~ 1 ps to 3 ns (depending on target position)
Ion energy	0.4 to ~ 40 MeV	0.5 to 16 MeV	0.8 to 1.2 MeV	~ 1 to 20 MeV
Ion peak intensity	Single ions to ~ 100 nA/mm ²	>10 A/cm ² , 0.1 to >10 J/cm ²	0.1 to 2 A/mm ² , 0.1 to 0.8 J/cm ²	0.1 to 1 μ A, 0.1 to >1 J/cm ² (with re-focusing)
Ion species	Protons to high Z	Protons, nitrogen, ...	He, other gases	Protons, carbon, noble gases (for gas jet), high Z
Examples presented	Tandems at Sandia, Single ended pulsed beam at LLNL	Hermes III, RHEPP-1 (Sandia)	NDCX-II (LBNL)	BELLA-i (LBNL), Laser+gas jet (SLAC)

In parallel to the development of pulsed ion beams as novel pump pulses, fast and ultra-fast structural probe techniques are also developing rapidly. X-ray free electron lasers are recognized as supreme probes of structural evolution with femto-second pulses. Techniques based on fs-laser driven coherent acoustic phonons have recently been applied to the spatio-temporal tracking of radiation damage. And recently, ultra-fast electron diffraction technology has been advanced to the (sub-) 100 fs level. Talks describing new UED instruments at LBNL and SLAC highlighted status and performance potential of this technique. Recent results from SLAC showed measurements of structural evolution in the melting of pre-damaged gold with unprecedented precision. The instrument at LBNL is coming online and is designed for a unique repetition rate up to 1 MHz. For the first time, this promises to make direct contact to extended simulations on the micro-second time scale. Both tools are ripe for pairing with pulsed sources to excite structural dynamics, such as ion beams and pulsed plasmas, to complement the currently used fs-lasers. Discussions highlighted the exciting opportunities warranted by pairing of pulsed ion beams and pulsed plasmas with a UED structural probe to access the dynamics of radiation effects across 15 orders of magnitude in time (from fs to seconds). Here, the significant challenges imposed by detector technology and data management could only be briefly touched on.

A talk on laser-plasma acceleration as a source of MeV electron pulses showed data that highlighting the prospect of single digit femtosecond time resolution of UED. Here, a synchronized pulse of laser-accelerated ions could be intrinsically synchronized to the UED probe, giving access to the femto-second time scale of collision cascades – perhaps the outstanding grand challenge of radiation materials science that would put widely used models to the ultimate test. These developments are also

exciting because they promise to inform theoretical studies that can link multi-scale processes in coupled electronic and lattice structure evolution and they can connect to rapidly developing techniques that probe electronic structure evolution (where one example is ARPES, angle resolved photoemission spectroscopy). A summary of (ultra)-fast probe techniques is given in Table 2.

Table 2: Examples of fast structural probes

	Transmission electron microscopy	Ultrafast electron diffraction	X-ray FEL
Probe pulse length	images with ~10 ms resolution (ns time scale in 4D electron microscopy)	~5 to 100 fs	<10 fs
Probe energy	~100 keV	0.1 to 5 MeV	0.4 keV to ~20 keV
Repetition rate	up to ~100 Hz image rate	0.1 KHz, 1 KHz, up to MHz	120 Hz
Examples presented	LBNL, Sandia	LBNL, LOA, SLAC	SLAC

The participants exuded a sense of excitement and anticipation in their talks and in the discussions. The workshop has served to highlight new experimental capabilities that promised to connect to and in some cases challenge theory and simulations and advances in simulation techniques that promises to soon enable direct benchmarking with multi-scale experimental results. Our workshop was made possible by leaders in radiation effects research who presented a cross-section of the field. While a remarkable range of perspective was present, not everyone invited could attend. One possible follow-up is to organize a session at a leading conference in this topic area (e. g. MRS Fall meeting).

Attendance metrics

- 45 registrants (some with dual appointments, some participated through a remote access link)
- US National Laboratories: 35
 - LBNL: 17
 - LLNL: 7
 - LANL: 2
 - ORNL: 1
 - PPPL: 2
 - Sandia: 4
 - SLAC: 2
- US Universities: 9
 - Rutgers University: 1
 - Stanford: 1
 - UC Berkeley: 3
 - UC Davis: 1
 - UC LA: 1
 - University of Tennessee: 2
- Other institutions: 3
 - Laboratoire d-Optique Appliquée, France: 1
 - GSI, Darmstadt, Germany: 1
 - University of Helsinki: 1

Topics and Speakers

Workshop on Dynamics of Radiation Effects in Materials

LBL, 15 - 16 December

Welcome and workshop goals, Wim Leemans and Thomas Schenkel

Dynamic Defect Production and Recombination Phenomena in Materials, Steve Zinkle, University of Tennessee

The challenges of Plasma Material Interactions in the fusion nuclear environment, Juergen Rapp, ORNL

Radiation defect dynamics studied by pulsed ion beams, Sergei Kurcheyev, LLNL

How reliable is molecular dynamics in predicting the time evolution of collision cascades? Kai Nordlund, University of Helsinki

Observation of ultrafast melting and bond softening in radiation damaged tungsten, Siegfried Glenzer, SLAC

Thermodynamics and kinetics of irradiation induced defects in nanocrystalline pyrochlore, Yong Wang, LANL

Characterization of the dynamics of surface morphology and nanostructure growth through spectroscopic ellipsometry and ion beam techniques, Robert Kolasinski, SNL

Transient Effects in Ion Irradiation, Len Feldman, Rutgers

Mesoscale modeling of irradiation damage processes in fusion reactor materials: a computational grand challenge, Jaime Marian, UCLA

New modes of electron microscopy for materials science enabled by fast direct electron detectors, Andy Minor, UC Berkeley and LBNL

Can Single Ion Strikes be Directly Observed in Relevant Time and Length Scales? Kahlid Hattar, SNL

Intense, short pulsed ion beams to access the dynamics of radiation effects, Peter Seidl and Arun Persaud, LBNL

working dinner at China Village, topic: emerging opportunities to benchmark models with pump-probe techniques, Thomas Schenkel

High Flux UED: challenges and opportunities, Daniele Filippetto, LBNL

kHz relativistic electrons driven by single-cycle laser pulse and their application to ultrafast electron diffraction, Aline Vernier, LOA

Operational Experience and Concerns Regarding Material and Equipment
Radiation Damage at the Los Alamos Neutron Science Center Target Facility,
Eron Kerstiens, LANL

Intense, short pulsed ion beams from laser-plasma acceleration to access the
dynamics of radiation effects at BELLA-i, Qing Ji and Sven Steinke, LBNL

Materials challenges for extreme radiation environments, Marilena Tomut,
GSI/FAIR

Effects of Electronic Energy Loss on Dynamics of Radiation Effects in Ceramics,
William J. Weber, University of Tennessee and ORNL

Exposure Effects due to Pulsed Intense Ion Beams: Radiation Effects (Hermes
III) and Mechanical Effects on Candidate Fusion First-Wall Materials
(RHEPP-1), Tim Renk, SNL

Demonstration of a <20 ns, High Flux Fast Pulsing Capability at Sandia's Ion
Beam Laboratory for Hostile Relevant Threat Environment Testing, Ed
Bielejec, SNL

Pulsed plasmas for pump-probe experiments, Andre Anders, LBNL

Small scale mechanical testing evaluating the impact of Helium on materials,
Peter Hosemann, UC Berkeley

Study of Lattice Motion in Ultrafast Laser Excited Non-equilibrium Warm Dense
Gold Thin Films, Zhijiang Chen, SLAC