Ion Irradiation and Computational Materials Science as Complements to Proton Irradiation for Advanced Beam-intercepting Device Materials Development

Letter of Interest for Snowmass 2021, Accelerator Frontier, Targets/Sources Subgroup

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Background

Existing proton accelerators, like the NuMI Beamline at the Fermi National Accelerator Laboratory (FNAL), utilize stainless steel and Al-base alloys for vacuum windows and graphite for neutrino-producing targets for high-energy physics research. The NuMI Beamline operated at 300 kW, but future experiments will require higher power proton beams to achieve neutrino production rates necessary to address physics such as matter-antimatter symmetry violation in neutrino flavor mixing. For example, the Long Baseline Neutrino Facility, planned for operation at FNAL and the Sanford Underground Research Facility in South Dakota, will utilize a 1.2 MW proton beam. Existing beam-intercepting device materials are unsuitable for use at this power because radiation damage will rapidly cause unacceptable degradation. Materials that are more tolerant to radiation damage are needed to enable adequate physics performance, acceptable lifetimes and cost-effective operation of high-power accelerators. Designers of future high-power accelerator windows and targets need to understand a variety of irradiation effects on materials including dimensional and phase stability, and thermal and mechanical property degradation. These effects are dictated by microstructural evolution caused by radiation damage to the crystal lattice of the materials. Thus, it is necessary to understand not only the macroscopic effects of radiation and its impact on material properties, but also the underlying radiation damage mechanisms that drive microstructural evolution.

An international team of researchers, under the aegis of the Radiation Damage In Accelerator Target Environments (RaDIATE) Collaboration, is in the midst of a series of high-energy (~180 MeV) proton irradiation experiments at the Brookhaven Linac Isotope Producer (BLIP) facility at Brookhaven National Laboratory (BNL). The test specimens include a variety of candidate materials for various beam-intercepting device applications and are provided by several accelerator facilities [1]. Post-irradiation examination, testing and characterization is being conducted at participating RaDIATE institutions with appropriate radiological facilities including Pacific Northwest National Laboratory (PNNL), FNAL, BNL and the Culham Centre for Fusion Energy. Of particular interest to the collaboration is irradiation and post-irradiation testing and characterization of Be, graphite, SiC-coated graphite, Ti-base alloys, Si, CuCrZr, Mo-TZM and Ir, which are candidate materials for targets, vacuum windows, beam dumps and collimators in current and future accelerator facilities planned by FNAL, KEK, CERN, and other organizations. Mechanical property data and microstructural characterization of Ti-base alloys irradiated in this series of experiments have recently been published and provide first-of-a-kind data for high-energy proton irradiation of these materials [2]. Additional publications on mechanical properties and microstructural evolution of Be are forthcoming.

The high-energy proton irradiation experiments at BLIP provide near-prototypic conditions for many beam-intercepting device applications, but they are expensive and take a long time. Planning for the first BLIP irradiation began in 2015 and the first publication of post-irradiation data was in 2020. While near-prototypic proton irradiation studies are necessary to obtain reliable engineering data to support device design, much can be learned from ion irradiation studies coupled with atomistic and meso-scale materials modeling about fundamental radiation damage mechanisms. This basic understanding can be used to guide materials selection and development and provide insight for planning more prototypic proton irradiation studies. A coordinated program of ion irradiations, proton irradiations and materials modeling will provide both engineering data and fundamental scientific understanding of radiation damage in candidate beam-intercepting device materials, and will enable future accelerator facilities that require more radiation damage tolerant materials.

Ion Irradiation

Ion irradiation has been extensively used as a tool to understand fundamental radiation damage in fission and fusion reactor materials [3,4]. Low-energy ion irradiations are attractive because they allow study of the microstructural evolution during irradiation without activating the specimens, are relatively low cost, and can achieve high dose in very short durations. One must be cautious, because ion irradiation damage effects are confined to a thin deposition layer (typically on the order of a few μm) and do not include gas production effects, although they can be mimicked by simultaneous or sequential hydrogen and helium ion implantation. This typically limits characterization to time-of-flight secondary ion mass spectrometry, transmission electron microscopy and atom probe tomography (and associated chemical and crystallographic analysis methods), but these are precisely the tools that can provide the desired atomic- to nm-scale insight while also providing data for direct comparison to atomic-scale simulations [5,6,7]. Comparisons of ion irradiation produced microstructures must be validated by comparison to prototypic proton irradiation produced microstructures and by adjusting the ion irradiation conditions to ensure the relevant damage processes are comparable. Keeping in mind the limitations, low-energy ion irradiations can be very helpful to help guide materials selection and design, and also to interpret results of high-energy proton irradiation damage studies.

Computational Materials Science

Atomic- and meso-scale modeling of radiation damage mechanisms is advancing in the field of nuclear materials [8]. Typically, these studies begin with first-principles approaches such as density functional theory to calculate input values needed for larger-scale atomistic simulations using techniques such as molecular dynamics [9,10]. Molecular dynamics simulations can provide fundamental property values such as solubility and diffusivity [11,12], which are input parameters useful for meso-scale techniques like phase field models where microstructural evolution effects can begin to be understood [13]. Given an understanding of microstructural effects, and validation by comparison with ion and proton irradiation data, it may be possible ultimately to incorporate these effects in macro-scale models using finite element or finite volume methods to predict engineering-scale behavior and properties [14]. Such multi-scale, linked simulations provide a stepping-stone approach to understanding the impact of atomic-scale radiation damage effects on microstructural evolution and ultimately macro-scale behavior and properties. While the computational techniques presently available are not mature enough to accurately predict complex alloy response at the macro scale, the capability of these techniques to provide fundamental insight is well established. With improved understanding of the fundamental radiation damage mechanisms responsible for driving microstructural evolution, it is possible to gain insight into materials selection and design that can help with downselection of options for future experiments or guide alloy development.

Recommendation

We recommend pursuing ion irradiation experiments and computational modeling closely coupled with the ongoing proton irradiation experiments underway at BLIP. Complementary studies such as these have been performed successfully for reactor materials as illustrated by references 5-7 and 9-14, and they have demonstrated significant technical and programmatic benefit by improving fundamental insight into important radiation damage mechanisms and their effects on irradiation performance. Ion irradiation and computational materials modeling both have well-understood limitations, but they also offer the ability to study a large number of samples in a short period of time at modest cost, while providing fundamental insights into radiation damage mechanisms in relevant materials for beam-intercepting devices in high-power proton accelerators.

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