Advanced modelling for High Power Targetry

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Background

Materials modeling to predict the effects of radiation damage in nuclear materials has been the subject of academic research since the 1950s and many advanced techniques have been developed since then and continue to be a highly active research area today. Techniques range from *ab initio*-based atomistic approaches to mesoscale (continuum) models that capture the materials microstructure to empirical correlations. The most fundamental of these (atomistic, molecular dynamics) have been successful in modeling local defect formation and clustering but they are limited in time-scale and length-scale of processes that can be captured by the model. Continuum methods (rate theory modeling, cluster dynamics, phase field) can offer results at the micro-scale for vacancy cluster formation and gas bubble growth and migration (as well as segregation of impurities to extended microstructural features, such as grain boundaries and dislocations). Although these mesoscale models take *ab initio* generated results as an input, they still require significantly difficult benchmarking and empirical correlation analysis. These types of simulations also need to be integrated with thermomechanical models that account for the coupled effects of specimen geometry, applied and residual stresses, and thermal history on the microstructure. Examples of coupling pursued in the nuclear materials community is combination of a phase field and crystal plasticity modeling. The crystal plasticity approach (which captures the behavior of material within a grain based upon direction dependent mechanical property measurements) is starting to incorporate grain boundary and impurity effects but is rooted in empirical measurements for derivation of strength and damage models.

As with the global radiation damage R&D program, fundamental material modeling of radiation damage expertise is held mostly in the nuclear materials communities at fission and fusion power focused laboratories and affiliated universities. Again, the large differences in irradiation environment parameters, especially dose rate and rapid thermal cycling, between accelerator targets and reactors greatly complicate the direct transfer of modeling techniques and correlations. As such, there have been relatively few attempts to model radiation damage effects from fundamental principles for accelerator target irradiation environments. It should be noted that radiation damage to electronics (relevant to space, satellite, and defense applications) is largely addressed as a separate issue, since the dose rates are several orders of magnitude lower.

The RaDIATE collaboration (Radiation Damage In Accelerator Target Environment) [2] led by Fermilab will coordinate the HPT R&D program between institutions who have expertise and common interest among the 14 international institution members.

Fundamental radiation damage effects material modelling

Fermilab started working with the University of Wisconsin's Computational Materials Group, led by Dr. Izabela Szlufarska, to understand the state of the art for fundamental material modeling

of radiation damage effects and how they could be incorporated into the HPT R&D program. Currently a research associate at UW-Madison has begun the first phase of a three-year project to develop a cluster dynamics/rate based model for helium gas bubble formation, growth, and migration in high-energy proton irradiated beryllium.
A number of modeling studies have been reported in the context of fusion research to understand behavior of radiation-induced defects and of He bubbles in Be. These modeling studies include atomistic simulations of fundamental properties of defects and continuum level modelling of He bubble evolution in irradiated Be. Atomistic simulations provide an excellent tool for understanding kinetic processes of radiation-induced defects and impurities and they are critical for providing parameters for continuum level models.

The project proposes to develop an experimentally validated computational framework capable of predicting radiation damage evolution in beryllium, which is a promising material for applications in the current and future particle accelerators. In particular, a proposed multi-scale model is focused on He bubble formation and growth as a function of irradiation temperature and on the contribution of these bubbles to swelling. In addition, the project proposes to carry out a series of targeted ex-situ and in-situ single and dual-beam ion irradiation experiments using low-energy protons at various temperatures and irradiation damage to provide critical data for validation of the model on the effects of radiation on He clustering, He bubble distribution, and dislocation loop density/size in proton irradiated Be.
The proposed model could eventually guide a choice of microstructures and alloys of Be and therefore would be greatly beneficial to the design and robust operation of accelerator target facilities.

The project will draw upon the previous RaDIATE collaboration irradiation studies of beryllium for empirical data to correlate/validate the resulting model. If successful, the model will allow scientists to predict the optimal irradiation temperature for beryllium targetry components to achieve maximum lifetimes by mitigating helium embrittlement and swelling.

Recommendation

The promise of material-by-design is very attractive and could eliminate costly experiment iterations for material development. Therefore, modeling efforts should be supported within the framework of HPT Materials R&D.