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Title: Radiation Damage from Atomic to Meso-Scales in Extreme Environments (REVISED)

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A foreboding materials challenge is to be able to withstand the 10–15 MW-year/m² neutron and heat fluence expected in the first wall and blanket structural materials of a fusion reactor.¹ Overcoming radiation damage degradation is a key rate-controlling step in fusion materials development. New science, approaches, and facilities are needed at multiple scales.

One of several new Energy Frontier Research Centers is one Los Alamos leads for “Materials at Irradiation and Mechanical Extremes.” Its objective is to understand, at the atomic scale, the behavior of materials subject to extreme radiation doses and mechanical stress in order to synthesize new materials that can tolerate such conditions. The understanding of fundamental unit mechanisms responsible for processes such as Frenkel pair recombination, defect clustering and precipitate nucleation, point defect interactions with interfaces, and dislocation core spreading are critical to the prediction and control needed for the bottom-up design of materials with unprecedented tolerance to extreme irradiation environments. The importance of interface structure in influencing these unit mechanisms operating at very small spatial scales cannot be over emphasized. Early work studying the interaction between point defects and grain boundaries (homophase interfaces)² confirm qualitatively that the response of different grain

boundaries to irradiation and impurity concentrations depends on interface structure³ and the presence or absence of coherency. However, because experimental and modeling methods were limited, the connections between modeling and experiments were necessarily qualitative in nature. The dependence of interface response to atomistic and collective processes occurring at extreme doses, dose rates, stress and temperatures were not investigated and remain poorly understood.

Improvements in computational resources and the advent of accurate inter atomic potentials have allowed atomistic modeling to provide greater insight to the connection between interface structure and response to irradiation. Figure 1 illustrates an example. Traditional structural materials degrade and fail under intense irradiation, but certain nanocomposites contain high volume fractions of “super-sink” interfaces that allow these materials to self-heal. Understanding how radiation damage is trapped and removed at such interfaces will help in designing a new class of radiation-tolerant materials that would make future nuclear reactors maximally safe, sustainable, and efficient. The Center is conducting both theory and experiment at these atomic scales that will be described. Other post-irradiation examination (PIE) being done includes tomographic radiography.

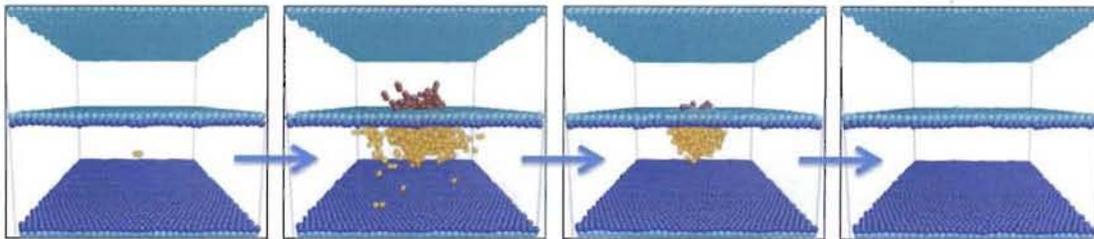


Figure 1: The time sequence (left to right) of radiation damage evolution near a super-sink interface formed by joining copper and niobium in a molecular dynamics simulation. Unlike in pure crystalline materials, the radiation-induced damage is completely absorbed by the interface. Similar effects are seen in post-irradiation examination of irradiated materials. Blue are interface Cu, gray interface Nb, yellow high-energy Cu, and red high-energy Nb in the CuNb nanocomposite material. All perfect fcc and bcc atom environments removed for clarity.

The Matter Radiation Interactions in Extremes (MaRIE) concept is a National User Facility to realize the vision of 21st century materials research and development. A key extreme environment for future energy security is intense radiation. Evaluation of radiation effects in a fusion environment requires simultaneous displacement damage (~200 dpa) and He generation (~2000 appm He) on multi-granular samples with properties of bulk material. Data without high fusion relevant dpa and He/dpa are of limited value. Evaluation of mechanical properties for a given material at a given temperature requires a minimum volume of ~10 cm³ with flux gradients < 20%/cm.

The Fission and Fusion Materials Facility (F³) segment of MaRIE proposes to use the present proton linac at Los Alamos with a power upgrade to drive a spallation neutron source that can provide the required radiation environment. Importantly, F³ would also provide the capability for *in-situ* measurements of transient radiation damage, using unique x-ray and charged particle radiography diagnostics. The mission of the facility would be to study material science in radiation extreme environments to provide predictive capability of material performance to allow certification of new nuclear systems. It is *not* intended for large-volume component testing. Scientific issues such as corrosion, strength and structural integrity, phase stability, thermal transport, and swelling in extreme radiation environments would be addressed. Coupled with integrated synthesis and characterization capability, the *in-situ* measurements with F³ would reveal not only the atomic scale origins of these effects but also their meso-scale consequences. The radiation environment possible (see Figure 2) with the current beam current of 16.5 mA and duty factor 7.75% or slight upgrades will be described.

¹ "R&D Needs and Required Facilities for the Development of Fusion as an Energy Source," Report of the Fusion Facilities Review Panel of the European Commission, October 2008.

² R. W. Siegel, S. M. Chang, and R. W. Balluffi, *Acta Metallurgica* 28 (1980) pp. 249. A. H. King and D. A. Smith, *Philosophical Magazine A*, 42 (1980) pp. 495.
³ A. Seki, D. N. Seidman, Y. Oh, and S. M. Foiles, *Acta Metall. Mater.*, 39 (1991) pp. 3167. A. Seki, D. N. Seidman, Y. Oh, and S. M. Foiles, *Acta Metall. Mater.*, 39 (1991) pp. 3179.

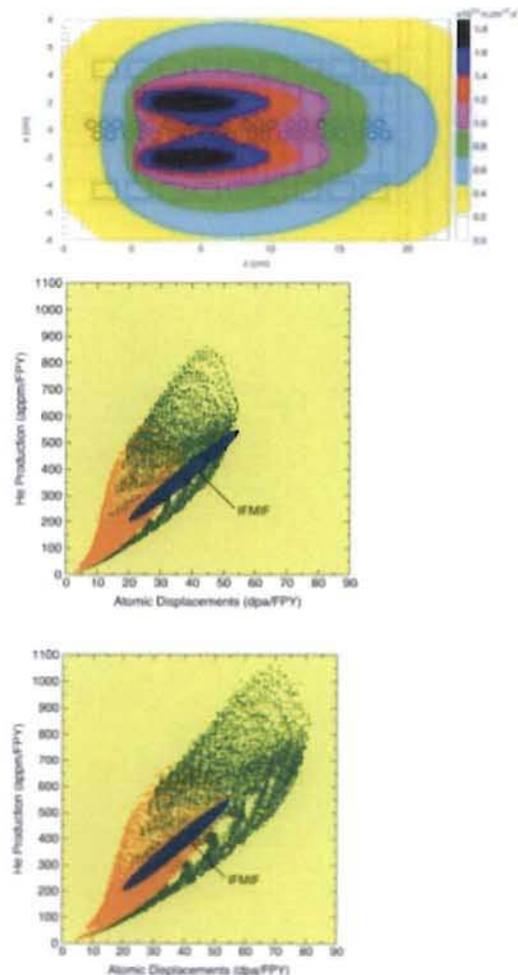


Figure 2: Radiation Environment for the proposed Fission and Fusion Materials Facility. a) Plan of the spallation neutron source, showing neutron flux contours at 1 MW level. b) He production vs atomic displacements at 1.8 MW, with each point representing a volume element in the source. The proposed IFMIF design space is shown for comparison. c) Same as b) but at 3.6 MW.

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