Atomic-Scale Design of Structural Materials for Fusion Environments

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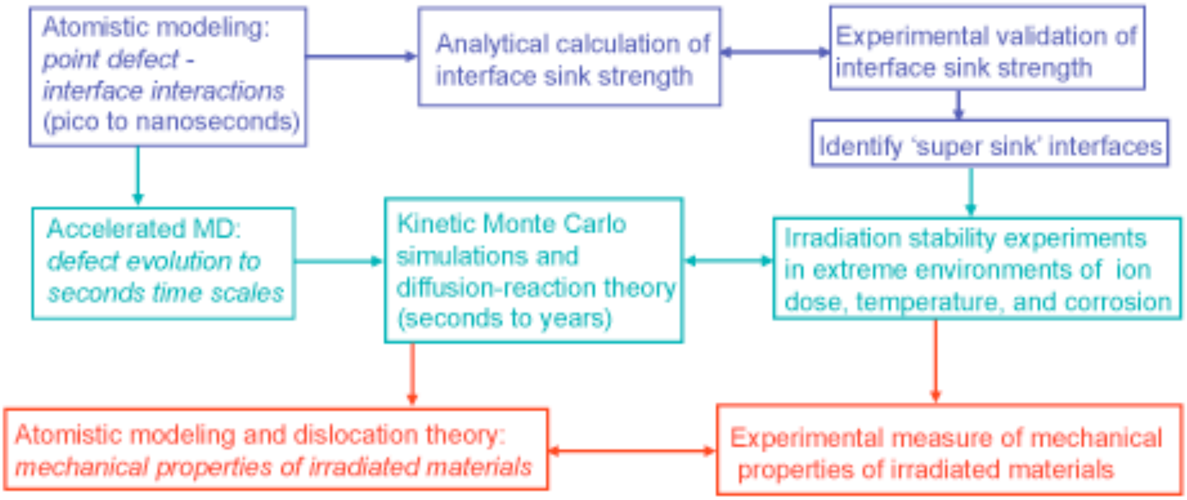
The report *Priorities, Gaps and Opportunities: Towards a Long-Range Strategic Plan for Magnetic Fusion Energy* submitted in October 2007 to the Fusion Energy Sciences advisory committee (FESAC) specifically calls for "*new science-based methods incorporating improved cross-cutting fundamental knowledge of basic radiation damage mechanisms in materials*" to the development of new materials "*capable of sustained high performance operation in extreme fusion environment*". This white paper directly addresses two of the seven scientific challenges outlined in the section 2.b.13 *Materials Science in the Fusion Environment* of the FESAC report. These two challenges / gaps in the current knowledge as called out in the FESAC report are: (i) experimental and modeling investigations of the stability (dimensional and phase) of new materials systems engineered at the nanoscale for superior radiation resistance. Void swelling and dimensional growth due to irradiation creep is expected to be much more in fusion reactors (≈ 10 appm helium/dpa) as compared to fission reactors (≈0.1 appm He/dpa). (ii) investigation of the mechanical properties of structural materials after radiation. The current knowledge base for the effects of radiation on the mechanical properties of structural materials is limited to ≈ 1 dpa and ≈ 10 appm, approximately 2 orders of magnitude below the projected operation conditions. The FESAC report calls for research on model as well as prototype material systems involving both experiments and multi-scale simulations that span from atomic dimensions to macro-scale and from pico-seconds to years.

This proposal is to develop material design principles for new nano-engineered material systems with predictive performance in extreme fusion environments using an integrated approach of experiments and multi-scale modeling. The objective is to be able to "predict" and "control" the material behavior as opposed to "observe and validate".

The hypothesis driving this "bottom-up" materials design approach is that perfect defect recovery implies perfect radiation endurance. The proposed approach is to create traps, such as interfaces, for residual cascade defects. Such traps function by virtue of high defect mobilities and high rates of recombination. 1-D fast migration of point defects in metals could enable new control of defect microstructures such as effective defect removal [1]. Furthermore, recent experiments and molecular dynamics (MD) simulations on a model Cu-Nb system suggest that nano-layered materials can derive unusual resistance to radiation damage because radiation-induced point defects cannot develop in the presence of high defect sink densities that interfaces in these materials provide [2,3]. After helium implantation at room temperature to a high dose (peak He concentration ≈ 5 at.%, DPA=9), transmission electron microscopy revealed that the individual 2.5 nm thick Cu and Nb layers remain distinct (no intermixing), and voids, gas bubbles, and other defect aggregates such as dislocation loops or stacking fault tetrahedra were not evident. *These initial MD simulations have shown that Cu-Nb interfaces are virtually inexhaustible sinks* *for both vacancies and interstitials, and have provided insights on the fundamental physics driving the role of interfaces in these materials in trapping defects*. First, the defect formation energies are significantly lower in the interface than elsewhere in the crystal (0.1-0.3 eV in the interface as opposed to 1-3 eV in bulk). Second, the range of interaction with other point defects, the so-called core size of trapped defects, is much larger at interfaces than bulk. Third, the defect mobility at interfaces is higher than in the bulk. Thus, the probability and the rate of defect recombination at interfaces are significantly higher than in bulk. These preliminary findings call for an in-depth study to understand how the interface properties (atomic structures and energetics) can be manipulated to enhance the absorption and annihilation of radiation-induced defects. The response of coherent and semi-coherent fcc(Cu) – fcc(Ni) interfaces to displacement cascades has also been studied at PNNL, where the defect yield at interface was found to be two-thirds of the average defect yield for cascades in bulk metals [4].

The preliminary findings stated above lead to two hypotheses:
(i) special interfaces can be designed to attract, absorb and annihilate radiation-induced point defects, and
(ii) nanocomposites containing a high volume fraction of such interfaces are expected to exhibit long-term morphological stability under elevated temperature irradiation. Based on these hypotheses, a new paradigm in the design of materials that are tolerant under extreme radiation environments is proposed.

To test these hypotheses, an example of the integrated experiments and multi-scale modeling research approach that is being pursued at LANL is summarized in the flow chart below.



Atomistic modeling will be used to study the interactions between interfaces and radiation-induced point defects. This will help in the development of a generalized, analytical model of the sink strength of interfaces that will allow calculation of a "figure-of-merit" for interfaces. These predictions of interface sink strengths will be validated via experiments on model systems with different values of "figures-of-merit". The outcome of this approach will be identification of

specific interface types that are best as sinks for radiation-induced point defects. Composite systems synthesized using these special interfaces can be subjected to irradiation stability experiments at high helium dose conditions anticipated in fusion environments. After irradiation, the mechanical properties such as strength and ductility will be measured to determine the extent of embrittlement after irradiation. To model the stability of interfaces at high helium doses at long times at elevated temperatures, accelerated MD and kinetic MC methods will be used, along with rate theory calculations. For a given distribution of radiation damage retained, atomistic modeling and dislocation theory will be used to model the radiation hardening.
While the atomistic modeling (and the initial experiments to test the modeling predictions) will be performed on metal-metal model systems such as Cu-W, etc for which accurate interatomic potentials are available, the predictions of the analytical models will enable design of prototypical systems such as nano-engineered steel composites [5]. In others words, *the knowledge base from this research can provide the scientific basis for first-principles driven atomic design of radiation tolerant multi-phase structural materials for fusion reactors*.

This multi-scale, integrated experiments-modeling approach requires state-of-the-art research facilities, which exist at National Laboratories and Universities throughout the US. As an example, LANL has Center for integrated nanotechnologies (CINT) for nanoscale synthesis, Ion beam materials lab (IBML) for ion irradiation and ion beam analysis, electron microscopy lab, and neutron scattering center for characterization of irradiated materials. Furthermore, LANL's upcoming signature facility MaRIE (Matter-Radiation Interactions at Extremes) will provide unique capabilities in irradiating and characterizing the ion-solid interactions at extremes. On the computational side, codes are being ported to perform accelerated MD in supercomputers (e.g., Roadrunner at LANL) to obtain boost in both length and time scales, e.g., micro-seconds to seconds at system sizes in excess of million atoms. Sub-Å resolution TEM capabilities exist in DOE user facilities at ORNL and LBL.

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