Center for Materials at Irradiation and Mechanical Extremes
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Lead Institution: Los Alamos National Laboratory

Mission Statement: 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.

Our EFRC addresses two of the five BESAC grand challenges: *How do we design and perfect atom and energy-efficient syntheses of revolutionary new forms of matter with tailored properties?; and How do we characterize and control matter away-especially very far away-from equilibrium?* In responding to these grand challenges our center will focus on *Materials at Irradiation and Mechanical Extremes (MIME).* This Center recognizes that the challenge to developing materials with radically extended performance limits at irradiation and mechanical extremes will require designing and perfecting atom- and energy-efficient synthesis of revolutionary new materials that maintain their desired properties while being driven very far from equilibrium. We have developed a set of common issues that will drive our science focus and serve as the unifying foundation of this center. These scientific issues include: 1) Absorption and recombination of point and line defects at interface; 2) Morphological and chemical stability of interfaces; 3) Interface-driven mechanical response. By addressing these issues we will develop a fundamental understanding of how atomic structure and energetics of interfaces contribute to defect and damage evolution in materials, and use this information to design nanostructured materials with tailored response at irradiation and mechanical extremes.

In the pursuit of the grand challenge and science issues outlined above, we have developed specific hypotheses for each science issue. These defining hypotheses are listed below.

Scientific issue #1: *Absorption and recombination of point and line defects at interfaces*

<u>Hypotheses</u>:

1) The atomic structure of the interface controls the absorption, emission, storage and annihilation of defects at the interface.

2) Misfit dislocation intersections with other misfit dislocations and with disconnections are the most favorable sites for point defect absorption and delocalization.

3) The lower the elastic strain energy penalty associated with defect absorption, the more likely it is that point defect delocalization by interface reconstruction can take place.

4) The ability of an interface to absorb dislocations is determined by its shear strength and the areal density of preferred sites for nucleation of interface glide dislocations.

Scientific issue #2: *Morphological and chemical stability of interfaces*

<u>Hypotheses</u>:

5) Interface structures with high sink strengths or enhanced abilities to act as defect sources will be morphologically stable at extremes of temperature, irradiation and mechanical deformation.

6) Interface energy controls interface stability; high-energy interfaces are less likely to be morphologically stable.

7) The saturation limit for defect absorption at interfaces for <u>a given type of defect</u> (e.g., helium atom, solute segregant, vacancy, interstitial, dislocation) is determined by the interface structure. Above the defect solubility limit, interfaces exhibit chemical instabilities such as defect clustering, gas bubbles, precipitates, disordering or amorphization.

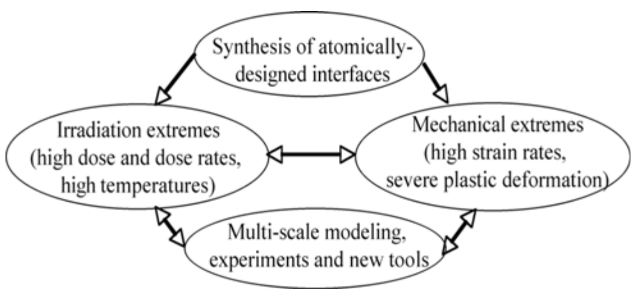
Scientific issue #3: *Interface-driven mechanical response*

Hypothesis:

8) The cohesive strength/mechanical damage evolution behavior for a given interface structure may change at high dose or high strain rates.

Using the above hypotheses, we have developed **quantitative figures-of-merit** for the defect sink strength of interfaces. These figures-of-merit will allow us to use a focused approach where model systems containing interfaces with high and low values of predicted sink strengths can be experimentally tested and the results used to refine the models.

The hypotheses driven research proposed in this center, will naturally have two focus areas (thrusts) dealing with the *role of interfaces* in: 1) *extreme irradiation environments*; and 2) *mechanical extremes*. Synergy will be enhanced through the development of new computational and characterization methods, and synthesis of common model systems. Materials will be synthesized via vapor deposition methods, solidification processing, diffusion bonding, and severe plastic deformation. Common theory, modeling, and simulation tools and methods will include *ab initio*, molecular dynamics (MD) and accelerated MD (AMD), kinetic Monte Carlo (KMC), rate theory calculations, and crystal plasticity modeling (large scale simulations will leverage LANL's supercomputer *Roadrunner*). New tools will be developed for extending our abilities to carry out multi-length and multi-time scale studies. This will include the development of a parallel off-lattice KMC, a hybrid MD/AMD/KMC method, and *in situ* ultra-fast laser and XRD characterization capabilities. The development of these methods will allow, for the first time, direct coupling of experimental measurements and computer simulations at comparable length and time scales. The integrated structure of the center is shown schematically in the figure below.



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