Center for Materials at Irradiation and Mechanical Extremes (CMIME)
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***Mission Statement**: To understand, at the atomic scale, the interactions of defects at interfaces in materials subjected to extreme radiation doses and mechanical stress in order to synthesize new interface-dominated materials that can tolerate such conditions.*

Our EFRC, the Center for Materials at Irradiation and Mechanical Extremes (CMIME), addresses two of the five BESAC grand challenges: (i) *How do we design and perfect atom and energy-efficient syntheses of revolutionary new forms of matter with tailored properties*?, and (ii) *How do we characterize and control matter away-especially very far away-from equilibrium*? In responding to these grand challenges our center focuses on designing structural nanomaterials for tailored response at irradiation and mechanical extremes. 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 interface-dominated materials where the atomic structures of the interfaces are used to tailor the interactions of point and line defects with interfaces and hence, the macroscopic material properties.

We have developed a set of common scientific issues that 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; and 3) Interface-driven mechanical response. We attempt to address these issues through a hypothesis-driven R&D approach that integrates experiments and theory. The key deliverables from this research program will be quantitative relationships between the atomic structure and energetics of interfaces and radiation or mechanical damage evolution in materials. These quantitative relations are *figures-of-merit* that can be used to rank different solid-solid interfaces in terms of the ability of an interface to control defect evolution.

Our center has two thrust areas in *irradiation extremes* and *mechanical extremes* respectively. The irradiation extremes thrust studies a range of radiation damage phenomena relevant to fusion and fission energy over a broad range of metal-metal, metal-oxide and oxide-oxide interfaces. The mechanical extremes thrust explores severe plastic deformation processing such as accumulative roll bonding (ARB) to design nanocomposites with interfaces that are crystallographically and morphologically stable at large plastic strains. The behavior of these ARB-processed nanocomposites is explored in a variety of conditions such as shock, high-pressure torsion, irradiation, fatigue, etc. Besides ARB, physical vapor deposition is used to synthesize model bi-layer or multi-layer systems for ion irradiation studies. Given the focus on mechanistic understanding at the level of atomic structure of interfaces, we study model systems such as Cu-Nb, Cu-Ag, $SrTiO_3$-TiO_2, etc where accurate interatomic potentials are available so that experimental results can be integrated with theory. For other more complex systems such as metal-oxide (Fe-Y_2O_3, Fe-TiO_2, etc) efforts are underway to develop charge-transfer based interatomic potentials. Likewise for long-time-scale simulation defect cluster evolution, method development activities involve atomistically-informed kinetic Monte Carlo approaches.

The progress in the development of *figures-of-merit* for interfaces is summarized in the following table.

Research Goals	Progress in the first 3 years
Understand helium storage at interfaces.	▪ Developed an equation that correlates the concentration of stored helium (He) at interfaces with the interface structure. ▪ Developed an equation-of-state for He bubbles at interfaces. ▪ Demonstrated suppression of material hardening due to He bubbles at interfaces. ▪ Collectively, the new understanding gained and the predictive capability that results will provide design principles for structural materials in fusion energy.
Understand sink efficiency of interfaces for radiation-induced point defects.	▪ Identified the types of point defect interactions at interfaces in terms of interface atomic structure and defect energetics and kinetics. ▪ Developed a model that accounts for the balance between irradiation conditions and recovery processes in nanoporous and multilayer materials.
Understand response of structure-less interfaces to radiation-induced point defects.	▪ Elucidated how point defects redistribute at interfaces in terms of defect energetics and kinetics. These results are being integrated into a predictive model that will enable the design of materials for fission energy applications.
Understand evolution of stable interfaces under severe plastic deformation.	▪ Discovered stable interfaces under accumulative roll bonding and developed theory for crystallographic and chemical stability of interfaces. Predictive capabilities are being developed.
Understand dislocation or twin nucleation at interfaces.	▪ Discovered deformation twin nucleation from specific interfaces in bulk accumulative roll bonding nano-composites. ▪ Identified how the interface structure affects defect (glide dislocation or deformation twin) nucleation at the interface. ▪ Initiated a predictive model, based on these results, which will provide the design principles for processing bulk nanocomposites for structural and nuclear energy applications.
Understand shock response of interfaces.	▪ Discovered varying shock response (e.g., stable or migrating boundaries, transgranular or intergranular spall) as a function of boundary structure. These results are being integrated into a predictive model that will enable the design of materials with a tailored response in high strain rate applications.

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