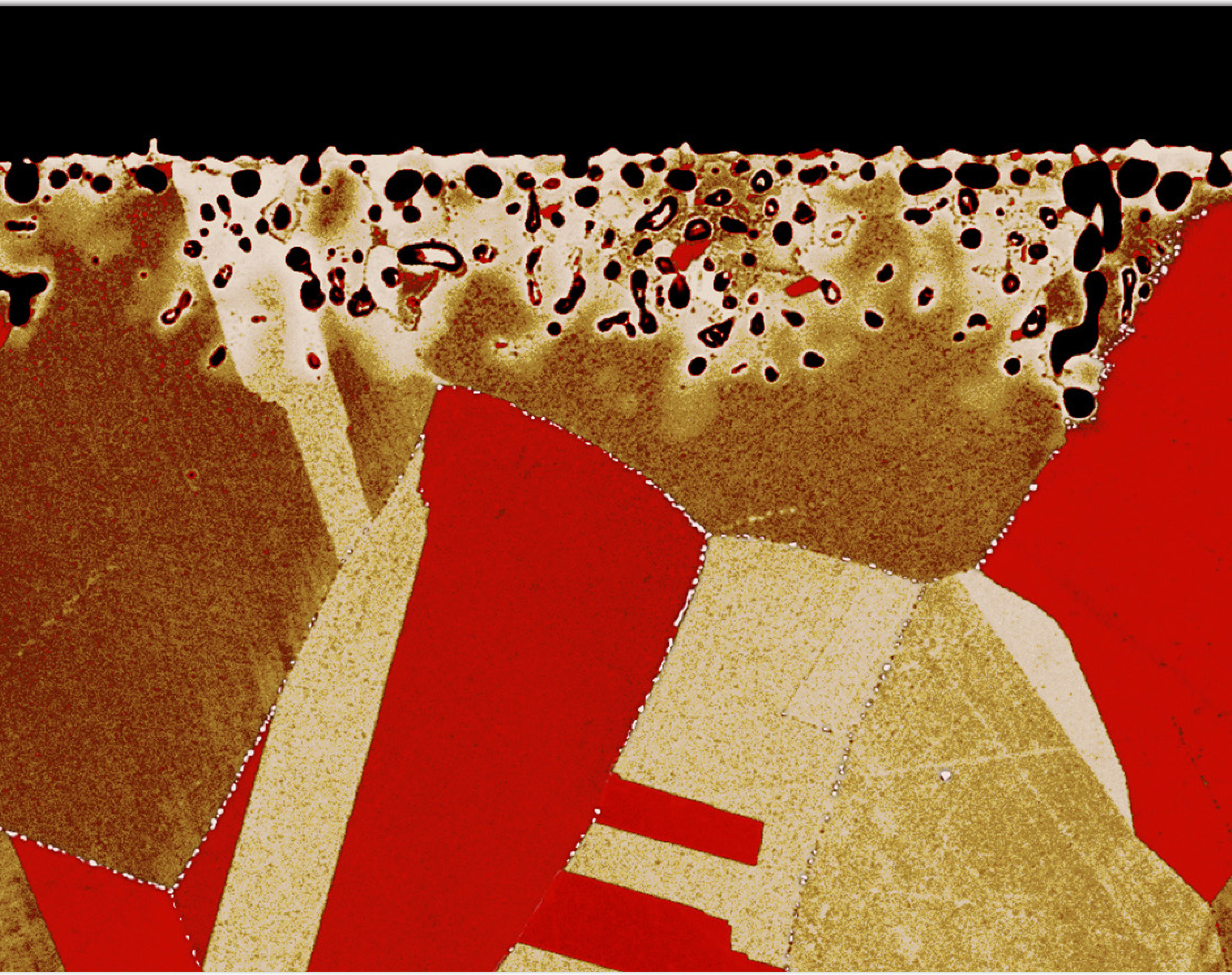
Basic Research Needs for

Future Nuclear Energy



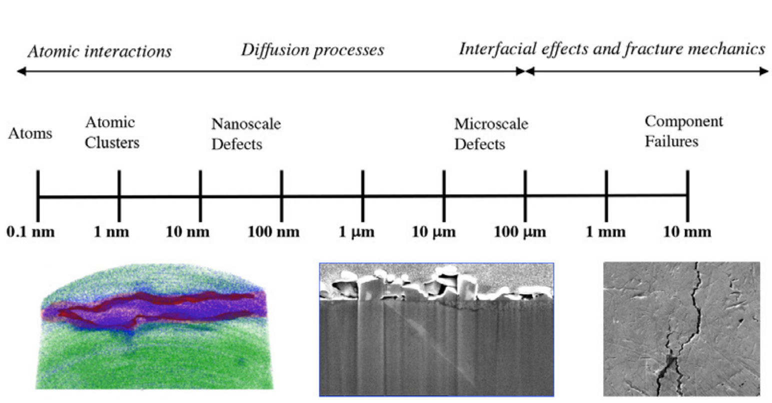
Future Nuclear Energy*—Inspiring Science at the Extremes of Chemistry and Materials*

Future Nuclear Energy—Realizing the full potential of advanced nuclear reactors

Concepts being developed for future, advanced nuclear reactors will go beyond producing an abundant, safe, reliable supply of electricity, to supporting lower-cost industrial production of materials and chemicals. However, realizing optimum future reactor concepts requires developing entirely different systems of coolants, fuels, and structural materials that can last through decades- to centuries-long reactor lifetimes and withstand some of the most extreme environments known—operational temperatures that could exceed 1000°C, intense radiation fields, and corrosive environments, among others.

These daunting requirements present an exciting and challenging opportunity for the chemical and materials sciences. They demand the discovery and design of revolutionary new materials and fuels, coupled with innovative approaches to materials synthesis and processing and optimization of the performance and certification of the new components. Combining modeling and simulation with in situ characterization methods will reveal and predict processes that dictate performance and degradation under extreme operational conditions. These coupled methods will also enable researchers to identify and understand the low-frequency events that can trigger cascading processes that may result in system failure. New computational tools and data analytics will expedite the identification of chemical compositions and structures of materials with tailored properties required to withstand the harshest reactor environments, followed by innovative synthesis and processing capabilities for materials production. Integration of the knowledge generated though this effort will accelerate the discovery-to-application process, providing the materials needed to realize the promise offered by advanced nuclear reactor concepts.

The report from a Basic Research Needs workshop held in 2017 identifies five priority research directions to understand the many physical and chemical processes underlying the performance of materials exposed to extremes of radiation, temperature, stress, and chemical reactivity. This knowledge is critically needed to design new materials and fuels for future nuclear systems. The full report will be available at https://science.energy.gov/bes/community-resources/reports/.



Physical and chemical processes in extreme environments including corrosion, oxidation, cracking, and fatigue span broad length and time scales from atoms (left) to components (right), which can result in degradation of desired properties and, ultimately, failures.

Images courtesy of Oak Ridge National Laboratory, Pacific Northwest National Laboratory, and University of Michigan.

Materials in nuclear reactors are exposed to some of the highest extremes in temperature, pressure, radiation, chemical reactivity, stress, and strain; and they must be designed to withstand these extremes for decades. Understanding and mitigating the mechanisms responsible for degradation is critical to meet the challenges for future nuclear reactors. Achieving this understanding requires information gleaned from experiments and modeling—from the atomic scale, to explain how atoms and molecules are arranged and may evolve, all the way to the mesoscale, to elucidate effects that result in macroscopic changes.

Priority Research Directions

- **Enable design of revolutionary molten salt coolants and liquid fuels**

  Key Question: *How can we characterize and predict the structure, dynamics, and energetics of molten salts—including an evolving chemical composition across length and time scales?*

  Molten salt coolants and liquid fuels are key elements in many future reactor concepts. During reactor operation, they exhibit a heterogeneous, evolving chemical composition, leading to large variations in structure, dynamics, and thermodynamics over broad time and length scales. New approaches are required to understand phase evolution and thermodynamics, including model systems to benchmark computational models, theories, and instrumentation.

- **Master the hierarchy of materials design and synthesis for complex, reactor environments**

  Key Question: *How do we design, synthesize, and process superior materials able to function and perform over decades in the extreme environments of advanced nuclear reactors?*

  Advanced reactor concepts place stringent long-term demands on structural materials and solid fuels. To realize these reactors, new computational- and data-driven approaches, along with innovative synthesis and processing methods, must be developed to accelerate discovery and enable production of material systems with functionalities tailored to withstand the operating environments.

- **Tailor interfaces to control the impact of nuclear environments**

  Key Question: *How can the multitude of inextricably linked chemical and physical processes that occur at interfaces be controlled?*

  Interfaces between materials and phases dominate the energy production infrastructure—from structural components exposed to liquid coolants, to the interior microstructures of constituent materials. Complex processes that occur at these interfaces must be understood and controlled to ensure long-term reliability.

- **Reveal multiscale evolution of spatial and temporal processes for coupled extreme environments**

  Key Question: *How can computational and experimental techniques be integrated to bridge spatial, temporal, and energy scales that underpin materials' behavior and chemical transformations in coupled extreme environments?*

  Many mechanical and chemical processes, especially in extreme environments, occur separately or in combination over wide time and length scales and degrade materials used in reactor systems. Experimental and computational capabilities must be integrated to reveal the processes that evolve over such broad temporal and spatial scales.

- **Identify and control unexpected behaviors from rare events and cascading processes**

  Key questions: *How do we identify, anticipate and control rare events that initiate cascading processes and cause aberrant properties and materials' responses?*

  In nuclear energy environments, high-impact, low-frequency events change material properties in ways that may ultimately lead to unexpected behaviors and even catastrophic failures. Variability in materials, impurity-controlled reactivity, sensitivity to radiation/radiolysis, localized transient behavior, and chemical evolution can act separately or synergistically to launch a cascade of unforeseen events. Scientific understanding of these conditions is central to the design of future nuclear energy systems.

Summary

Future nuclear reactor concepts will allow the realization of the full potential of nuclear energy as a reliable, sustainable energy source, generating clean electricity and supporting lower-cost industrial production of materials and chemicals. New coolants, fuels, and structural materials are needed to realize this potential. Developing them requires unparalleled improvements in the performance of materials and mandates an understanding of the physical and chemical processes that control and degrade the performance of materials.

The five priority research directions in the report identify the key scientific challenges that must be met to achieve a multiscale spatial and temporal understanding of fundamental processes that govern the performance of materials in the extreme environments envisioned for these reactor designs. New modeling and simulation, data analytics, synthesis and processing science, and in situ characterization capabilities will provide unprecedented insights to enable the design, discovery, and production of revolutionary materials, coolants, and fuels required for operation in complex, evolving harsh environments. The challenges and opportunities outlined in the report will build the scientific basis required to further the development of nuclear energy sources to meet the future energy needs of the nation.

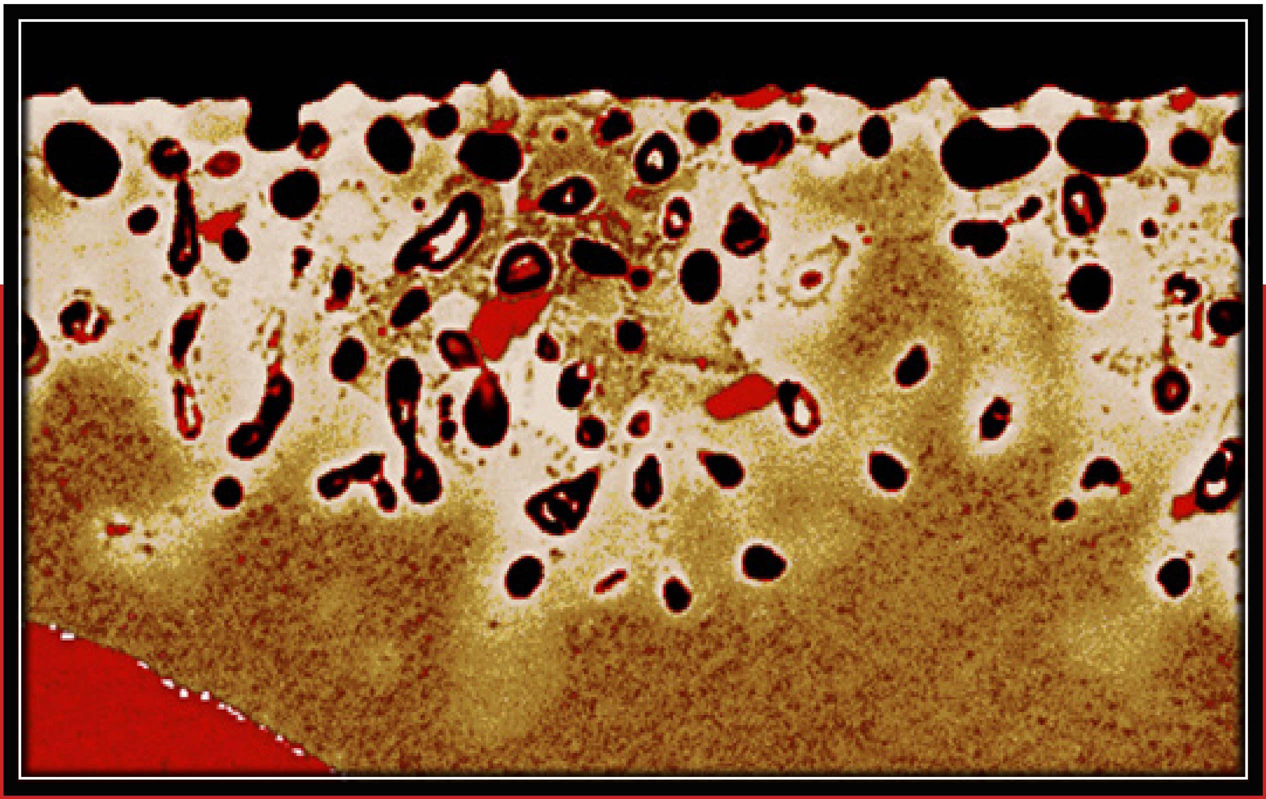


Image courtesy of Oak Ridge National Laboratory.

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