

**U.S. DOE ADVANCED MANUFACTURING OFFICE, OFFICE OF FOSSIL ENERGY,
AND OFFICE OF NUCLEAR ENERGY
MATERIALS FOR HARSH SERVICE CONDITIONS VIRTUAL WORKSHOP**

October 27-30, 2020

11 AM to 3 PM Eastern Time, each day

Plenary Sessions on Oct. 27, 28

**Breakout Sessions on Oct. 29, 30 (active participation by invitation only,
observer slots available)**



[Agenda](#)

[Scoping Document](#)

[Breakout Session Questions](#)

Purpose

This information is provided in advance of the October 27-30, 2020 Materials for Harsh Service Conditions Virtual Workshop, and consists of an **Agenda**, a **Scoping Document**, and **Breakout Session Questions**. The intent is to give participants an opportunity to prepare before arrival, and ensure a productive workshop.

The Agenda includes presentations by several materials engineering experts from stakeholder industries, followed by interactive, facilitated breakout sessions where workshop attendees are encouraged to contribute knowledge and information.

The Scoping Document provides a high-level overview of the current needs of materials technologies, and highlights some of the technical challenges and Research & Development (R&D) opportunities of next-generation materials for harsh service conditions (aka harsh environments), with special emphasis on enabling manufacturing methodologies. It consists of three major sections:

- Section 1 highlights the motivation for pursuing mid-TRL (TRL 3-6) R&D initiatives in the harsh environment materials field, offers a brief introduction on the applications in which materials with more resiliency are expected to have a high impact on energy savings, and outlines the goals of the workshop.
- Section 2 provides an overview of different energy applications and the associated materials challenges.
- Section 3 provides materials and technology development needs that complements the narrative laid out in Section 2.

The Breakout Session Questions will be pursued through facilitated sessions, and will include discussion on the merits of candidate technical targets for areas of interest to DOE.

Disclaimer

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U.S. DOE Advanced Manufacturing Office, Office of Fossil Energy,
And Office of Nuclear Energy
Materials for Harsh Service Conditions Virtual Workshop
October 27-30, 2020

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Materials for Harsh Service Conditions Agenda

Day 1 (Tuesday, October 27, 2020)	
11:00 am to 11:10 am	Workshop Administrative Team - Attendee Instructions and Expectations
11:10 am to 11:20 am	Welcome from the AMO Office <i>Ms. Valri Lightner, Deputy Director - Advanced Manufacturing Office, DOE</i>
11:20 am to 11:30 am	Workshop Background and Purpose <i>Dr. J. Nick Lalena, Technology Manager, AMO, DOE</i>
11:30 am to 11:35 am	Welcome from the Fossil Energy Office <i>Mr. Angelos Kokkinos</i>
11:35 am to 11:55 am	FE Office <i>Mr. Regis Conrad, Director of the High-Performance Materials Program</i>
11:55 am to 12:15 pm	Turbine Materials <i>Dr. Sean Bradshaw, Turbine Technology Manager, Pratt & Whitney</i>
12:15 pm to 12:35 pm	Low Carbon Resource Utilization <i>Neva Espinoza, Vice President Energy Supply and Low Carbon Resources, Electric Power Research Institute, EPRI</i>
12:35 pm to 12:55 pm	Coal to High Performance Carbon Products. <i>Mr. Charles Atkins, Ramaco</i>
12:55 pm to 1:15 pm	Materials and Manufacturing Challenges from a Supplier Perspective <i>Dr. Noah Phillips, ATI</i>
1:15 pm to 1:30 pm	BREAK
1:30 pm to 1:50 pm	Office of Advanced Reactor Technologies <i>Mr. Dirk Cairns-Gallimore</i>
1:50 pm to 2:10 pm	Harnessing Carbon Sources for Materials Production <i>Ms. Gay Wyn Quance, CEO-Solid Carbon Products</i>
2:10 pm to 2:30 pm	Topic of talk TBD. <i>Dave Gandy, EPRI</i>
2:30 pm to 2:50 pm	Digital Twin and Advanced Manufacturing Needs for Space Nuclear Technologies <i>Dr. Anthony Calomino, NASA</i>

2:50 pm to 3:10 pm	Carbon Composite and Carbides for Use In Advanced Reactor Systems. <i>George Jacobsen (General Atomics, Lead Scientist) Advanced Core Materials for Current and Next Generation Nuclear Reactors</i>
3:10 pm to 3:20 pm	Distributable Modular Nuclear Reactor Materials/Manufacturing Challenges. <i>Dr. Claudio Filippone, CEO-HolosGen</i>

Day 2 (Wednesday, October 28, 2020)	
11:00 am to 11:10 am	Workshop Administrative Team - Attendee Instructions and Expectations
11:10 am to 11:30 am	EERE Office Representatives <i>Mr. Alex Fitzsimmons, Deputy Assistant Secretary for Energy Efficiency, DOE; Dr. Dave Salon, Deputy Assistant Secretary for Renewables, DOE</i>
11:30 am to 11:50 am	EERE Solar Program <i>Dr. Avi Shultz, Solar Energy Technologies Office, DOE</i>
11:50 am to 12:10 pm	EERE Wind Program <i>Ms. Lillie Ghobrial, Wind Energy Technologies Office, DOE</i>
12:10 pm to 12:30 am	Hydrothermal and Low Temperature Resources <i>Dr. Alexis McKittrick, Geothermal Technologies Office</i>
12:30 pm to 12:50 pm	Hydrogen and Fuel Cell Technologies Office <i>Dr. Ned Stetson, Program Manager, Hydrogen Technologies</i>
12:50 pm to 1:00 pm	BREAK
1:00 pm to 1:20 pm	AMO Overview <i>Ms. Valri Lightner</i>

1:20 pm to 1:40 pm	Materials Challenges and R&D Needs for Harsh Environment Manufacturing Processes <i>Dr. Leo Christodoulou</i>
1:40 pm to 2:00 pm	Steel Industry Materials Challenges <i>Michael Sortwell, Senior Director, Technology, American Iron and Steel Institute.</i>
2:00 pm to 2:20 pm	A Diversified Industry's Perspective <i>Dr. Mark Thompson, Technology Leader, Cores and Castings, GE Power.</i>
2:20 pm to 2:40 pm	<i>Integrated Computational Materials Engineering and its application to the design and development of advanced engineering materials and materials for harsh service conditions</i> <i>Dr. Jason Sebastian, QuesTek</i>
2:40 pm to 3:00 pm	Materials Challenges with Industrial Gases & Chemicals <i>Max Christie, R&D Director-Ceramic membranes, Linde</i>
3:00 pm to 3:20 pm	Ceramics and High-Performance Materials <i>Dr. Anne B. Hardy, Vice President of Research and Development – High Performance Materials, Saint-Gobain</i>

Day 3 (Thursday, October 29, 2020)

11:00 am to 3:00 pm	BREAKOUT SESSION #1: Materials for Extreme Temperatures, Thermal Management, and Energy Conversion (4 hrs.) <i>Session Leads: Dr. Jeff Hawk (NETL), Dr. Kashif Nawaz, (ORNL)</i>
11:00 am to 3:00 pm	BREAKOUT SESSION #2: Wear, Oxidation, and Corrosion-Resistant Alloys, Components, and Coatings for Static and Rotary Applications (4 hrs.)

	<i>Session Leads: Dr. Bruce Pint (ORNL), Prof. Brian Gleeson (University of Pittsburgh)</i>
11:00 am to 3:00 pm	<p>BREAKOUT SESSION #3: Ceramics, Composites, and Functionally Graded Materials for Harsh Environments (4 hrs.)</p> <p><i>Session Leads: Dr. Edgar Lara Curzio (ORNL), Prof. Elizabeth Opila (University of Virginia)</i></p>

Day 4 (Friday, October 30, 2020)	
11:00 am to 3:00 pm	<p>BREAKOUT SESSION #4: Enabling Materials through Advanced Manufacturing Technologies (4 hrs.).</p> <p><i>Session Leads: Dr. Gary Rozak (HC Starck), Dr. Isabella Van Rooyen (INL)</i></p>
11:00 am to 3:00 pm	<p>BREAKOUT SESSION #5: Accelerating Qualification of Advanced Materials & Experimental Validation of ModSim Methodology for Materials, Manufacturing, and Performance During Service (4 hrs.).</p> <p><i>Session Leads: Dr. Dave Alman (NETL), Dr. Michael McMurtrey (INL)</i></p>
11:00 am to 3:00 pm	<p>BREAKOUT SESSION #6 ROUND TABLE: Mechanisms for collaborative demonstration of processes at industrially relevant scale (4 hrs.).</p> <p><i>Session Leads: Dr. Briggs White (NETL), Dr. Rob O'Brien (INL)</i></p>

Materials for Harsh Service Conditions Scoping Document

1. Introduction

The Department of Energy prioritizes intradepartmental collaboration to advance crosscutting initiatives. One recent intradepartmental collaborative opportunity involves advancing the development of next generation harsh environment materials. Harsh environments include exposures to: extreme or cyclical temperatures, pressures, mechanical wear/stress/strain/shock; chemicals and corrosive media (liquids and gases, including hydrogen), particulate loads; or radiation that constrain design choices and/or materials selection. Harsh environments can impede device operation and shorten a material component's useful lifetime. The **Harsh Environment Materials Initiative** (HEMI) was launched in FY2020 and was again included in the President's FY2021 Budget Request to Congress for the Department of Energy to meet the challenges of today and tomorrow by promoting energy independence, progressing scientific research, and protecting the Nation. Specifically, this cross-cutting activity between the **Office of Fossil Energy** (FE), the **Office of Nuclear Energy** (NE), and the **Advanced Manufacturing Office** (AMO) exploits synergies in materials and component manufacturing research for thermoelectric power plants.

Additionally, AMO's mission is to *catalyze research, development and adoption of energy-related advanced manufacturing technologies and practices to drive U.S. economic competitiveness and energy productivity*. Therefore, in this workshop the focus will be on high-impact opportunities to advance materials and materials manufacturing process technologies that improve system energy efficiency/performance and extend useful life where harsh service conditions exist, in electrical energy producing and in energy-intensive processes. Energy savings in these end-user applications can be of several forms: reduced embodied energies of material components used under harsh service environments; greater system/process energy efficiencies obtained through employment of material components with enhanced properties/performance; or savings via the use of a more resilient material with an extended service life under harsh service conditions.

Through this workshop and a recently released Request for Information (RFI), AMO, FE, and NE seek to gather input from stakeholders on the technical and commercial prospects of novel harsh service material development and new manufacturing capabilities. These include - but are not limited to - the advantages and technical challenges associated with new material breakthroughs, strategies for de-risking the cost and performance of novel materials, and considerations for scale-up of new materials manufacturing methods. Information is needed to set high-reaching targets/metrics and to identify the key problem sets to be addressed. The intent is to define critical crosscutting problems/barriers whose solutions represent **near-term commercially viable paths** to obtaining materials that can produce a step change improvement in energy performance under harsh service conditions beyond current state of the art.

The following objectives for the joint AMO-FE-NE workshop have been established.

- Identify high-value, cross-cutting research opportunities of interest to AMO/FE/NE related to materials challenges. Determine the research needed to overcome those challenges that prevent transition of the material into achieving improvements in energy efficiency or extension of service life of process componentry employed under harsh service conditions.
- Identify high-value, cross-cutting research opportunities of interest to AMO/FE/NE related to fabrication of operable parts/coatings. Identify advanced manufacturing research and methodology improvements needed that lead to reduced embodied energy in functional parts and coatings, improves material performance, operational service life, and achieves reduction in energy needed to operate the process under harsh service conditions.
- Identify material science data gaps and research needs that can lead to scalable, manufacturing techniques that give rise to parts and/or coatings whose physical properties and cost/value outperform conventionally produced parts.
- Identify opportunities, data gaps, and technical limitations preventing development of rapid qualification methodologies that reduce material/part certification time and cost.
- Identify data gaps and research needs that enable improvements in modeling/simulation methodologies for materials during fabrication and during operation under harsh service conditions at relevant spatial and temporal scales.
- Identify data gaps and research needs in fabrication process monitoring, control, and feedback that allows more efficient machine learning that translates to reduction in fabrication time, intensification of fabrication processes, and overall improvements in fabrication process efficiency.

These objectives will be expanded on in the next two sections of the scoping document.

2. Energy Applications and their Material Demands

It is widely recognized that many energy producing and energy-intensive technologies involve exposure of diverse material components in processes equipment to harsh conditions of some type (often, multiple types simultaneously) while in operation. Examples include: combustion chambers, gas turbines, steam turbines, wind turbines, furnaces, heat recovery systems, nuclear reactors, transportation, mining, oil & gas drilling equipment (on-shore and off-shore), as well as agricultural, primary metals, pulp and paper, chemicals/refining, and even food processing industries. The harsh environments in these applications represent extremes in temperature, pressure, chemical reactivity/corrosivity, mechanical erosion/wear/friction, particulate load, and radiation. All types of hard and soft materials are encountered: metals, ceramics, semimetals, semiconductors, composites, polymers, and amorphous/glassy substances. However, while considering the electrical energy production and energy-intensive applications discussed below, it is convenient to partition the technology space not by material type but rather by different types of harsh environments, for example, thermal, corrosive/chemical, and mechanical conditions, and by degradation mechanism (see Table below).

Harsh Environment ^A		Degradation Mechanism / Effect ^{B, C}
Thermal	Extremely High Temperature	Phase Stability
	Extremely Low Temperature	Embrittlement
	Other.....	
Thermal-Mechanical	Thermal Cycling	Fatigue
	Thermal Gradient	Dimensional stability
	Combined Thermal & External Mechanical Loading	Creep
	Other.....	
Mechanical	High Strain Rate	Ductility / Energy Dissipation
	Extreme State/Magnitude of Stress	Mechanical Failure / Overload
	Mechanical Interaction / High Friction	Wear, Galling
	Cycling / Loading History	Fatigue
	Other.....	
Mechanical-Chemical	Many...	Stress Corrosion Cracking
		Corrosion Fatigue
		Fretting Corrosion
Chemical	Salt Water	Various forms of Corrosion
	Raw Water	Microbiologically Induced Corrosion
	Industrial Gases	Hydrogen Embrittlement
	Industrial Liquids	Dealloying
	Industrial Solids	Solid Metal Embrittlement
Radiation	Nuclear Power Plant	Neutron Embrittlement
	Other.....	

^A Harsh environments are binned based on driving energy. Examples environments are provided for each bin.

^B Only one possible degradation mechanism or aging effect has been provided for each example environment.

^C It is not expected that all environments and degradation mechanisms are applicable to this workshop, for example, high humidity may be deleterious for electronic devices.

2.1 Fossil Energy Applications.

The Office of Fossil Energy's (FE) mission is to discover and develop advanced fossil energy technologies to ensure American energy dominance, create American jobs, support a resilient infrastructure, maintain environmental stewardship, and enhance America's economy. FE ensures America's access to and use of safe, secure, reliable, and affordable fossil energy resources and strategic reserves. Within FE, the Advanced Energy Systems (AES) program office focuses on improving the efficiency of fossil fuel-based power systems, transforming fossil energy systems for the future to enable highly flexible and reliable power systems with carbon-neutral emissions, pursuing new products from coal and captured CO₂, and accelerating pathways to valuable products via fossil fuel-produced carbon neutral-hydrogen.

Fossil fuel based power systems are high temperature processes. Maximum operating temperatures of these devices as well as other high temperature industrial processes are limited by their design, including the high-temperature phase stability and thermomechanical properties of the materials used in end-user component products and in process equipment, respectively. Opportunities exist to develop new high-performance, low cost materials as competitive and viable alternatives to traditional materials used in high temperature applications.

New materials with superior resistance to high-temperature oxidation, reduction, creep, fatigue, and phase transformation are needed for energy production, as well as in the energy-intensive transportation and industrial end use applications. Although it is impossible to define material property or performance criteria that are universally-applicable across all classes of materials and operating conditions or environments, very generally either steady-state creep (static loading), constrained or unconstrained thermal fatigue (cyclic loading), stress corrosion cracking, oxidation, reduction, phase transformation, decomposition, spallation, or undesired microstructural changes (e.g., coarsening) generally becomes a concern with metals, ceramics, and polymers beginning at some temperature range/interval. For example, as a general rule, creep occurs in metals when they are required to operate at temperatures above 30 to 40% of their absolute melting point, in polymers at 30–40% of their glass transition temperature, and in heat-resistant ceramic materials starting above 40–50% of their melting temperature.¹

A prominent example of a high temperature energy production technology that the DOE has funded research for is the gas turbine engine, which uses air as the working fluid. In a gas turbine engine, compressed air is drawn into the combustor along with fuel (natural gas) where the mixture is burned. The energy released from the fuel is absorbed by the air, which is passed into the turbine where the energy of the moving hot fluid is converted to mechanical energy that can be used to drive a generator to produce electrical power. Unconverted energy is exhausted as heat which may be recovered. Historically, increases in the thermal efficiency of this process have been achieved with increases in the initial temperature of the working fluid

¹ "Introduction to Aerospace Materials," A. P. Mouritz, Ed. Woodhead Publishing, Cambridge, UK (2012).

coming into the turbine from the combustor by making the fuel-air mixture in the combustor more fuel rich. The turbine components (blades and vanes) must possess superb high temperature mechanical properties, particularly high temperature creep resistance, as well resistance to cyclic loading. Fatigue is a common failure mode for gas engine turbine blades. Under fluctuating or cyclic stresses, failure can occur at loads much lower than the yield strength of a material under static load. In modern gas turbines, turbine inlet temperatures exceeding 1400°C are accomplished with nickel-based superalloys, single-crystal blades, thermal barrier coatings, and, of course, appropriate cooling mechanisms. Further increases in turbine inlet temperature will require turbine materials with superior mechanical properties (e.g. creep resistance, fatigue strength), high-temperature oxidation/corrosion resistance, and higher melting points, which limit further advancements in the operating temperatures and efficiencies of gas turbines using with metallic turbine materials. Carbon-based materials, carbides, and composites are of wide interest for use in this application.

When it comes to the efficiency of other fossil fuel based power plants, the same is true, the higher the pressure and temperature of the working fluid entering the turbine, the higher the efficiency. Because of this, steam turbine materials, for example, need to have excellent oxidation resistance in steam, as well as adequate creep strength, low thermal expansion, and high thermal conductivity, particularly advanced ultra-supercritical (AUSC) and supercritical CO₂ (sCO₂) systems.² The economic costs of materials corrosion (high temperature oxidation can be considered one type of corrosion) can hardly be overstated, as corrosion presents a significant challenge in nearly every industrial sector. In the energy industry corrosion-related failures can result in service outages. In energy-intensive industries (steel, chemical, petrochemical, etc.), process disruptions caused by component failures, necessitate startup/shutdown cycles that result in productivity loss and energy loss, especially in high-temperature production processes. The performance improvements needed for operation in corrosive environments call for chemically and mechanically robust materials that can economically replace traditional alloy materials as a promising route towards accelerated materials development.

Degradation mechanisms and performance criteria are naturally highly dependent on the specific features and properties of the material, as well as its service environment conditions. Therefore, as with high temperature environments, it is very difficult to define universally-applicable performance criteria for materials exposed to corrosive environments. High temperature corrosion or oxidation is normally discussed under high temperature phenomena.

² "Research and Development of Heat-Resistant Materials for Advanced USC Power Plants with Steam Temperatures of 700 °C and Above," F. Abe, *Engineering*, Vol. 1, Issue 2, pp. 211-224 (June, 2015).

2.2 Nuclear Energy Applications

The Office of Nuclear Energy (NE) has a mission to advance nuclear power to meet the nation's energy, environmental, and national security needs. Within NE, the Advanced Methods of Manufacturing (AMM) program goal is to accelerate innovations to reduce cost and schedule for new nuclear plant construction and to make fabrication of nuclear power plant components faster, less expensive, and more reliable. Paramount to achieving these goals is the development of materials that possess a number of attributes, including: superior stability against degradation from thermal and radiation exposure, as well as corrosive environments; materials which are dimensionally stable; and those which can be joined to dissimilar materials. Graphite, carbon composites, and carbides are materials of growing interest in nuclear reactor applications.

Alloy embrittlement is most directly associated with a loss of a material's ability to absorb strain energy. Embrittlement may result from penetration into the material by neutrons (radiation), as well as hydrogen, service fluids, or liquid nitrogen in the case of cryogenic processes. An alloy's susceptibility to embrittlement in a service environment can overly constrain design, decrease service life, and result in increased maintenance/inspection requirements. Preventing or minimizing embrittlement during processing/manufacturing can result in additional steps or controls, often resulting in higher embodied energy.

2.3 Renewable Energy and Manufacturing/Industrial Applications

The renewable energy sector is not immune from harsh service conditions and its adverse effects. Extremes in thermal gradients and corrosion from thermal fluid media are encountered in concentrated solar power systems. Wind turbines experience extreme and cyclical loads. Geothermal energy production has extreme temperature requirements. The consideration of harsh environments in manufacturing is dual-focused. Firstly, manufacturing processes produce the material components used in energy production and energy-intensive industrial applications and new more effective and more energy/cost efficient manufacturing methodologies (e.g. additive manufacturing) are needed to produce advanced materials able to withstand harsh environments. Secondly, as is so with the energy production technologies, many energy-intensive manufacturing industries (e.g. steel production, chemicals and refining, pulp & paper, etc.) involve a variety of harsh service conditions. These include high temperatures, corrosion, and embrittlement, which have already been discussed. Another type of harsh environment is mechanical wear. For example, the global estimate for contact friction and wear losses (as a percentage the total energy consumed) for the industrial sector (including mining, agriculture, primary metals, pulp and paper, chemicals/refining and food processing) has been estimated at around 20%.³ Paths are needed to reduce friction and wear losses in

³ Holmberg, K.; Erdemir, A. "Influence of tribology on global energy consumption, costs and emissions," *Friction* 5(3): 263–284 (2017).

such energy-intensive and high mechanical load applications, such as those found in the agricultural equipment, primary metals, pulp and paper, chemicals/refining and food processing industries. These may involve dynamic friction coefficients > 0.01 , and/or nominal contact pressures > 2 GPa. Additionally, information is sought on materials and manufacturing of sensors and other components suitable for sustained and reliable operation under conditions of high static and dynamic pressure (> 240 MPa), for example, in mineral extraction, well drilling, hot or cold isostatic processing, or other heavy-duty industrial processes.

3. Material and Manufacturing Technology Challenges and Opportunities

There is a wide array of advanced techniques to pursue materials that can handle harsh service conditions. Technology and application areas might include bulk material engineering (e.g. alloy development, engineered residual stress, phase change materials, and optimized micro/macrostructures); coatings; and sensors for in situ monitoring. A major goal is the identification of cost-effective, scalable, repeatable manufacturing methods (e.g., production and synthesis and surface engineering) for producing materials used that afford a high degree of microstructural control, and/or that can provide for the component geometrical designs required in energy applications (e.g. curved turbine blades). The material innovations can be discovered using high performance computing or other advanced techniques. They can be manufactured using additive manufacturing, among other methods.

3.1 Historical Context

Crosscutting fundamental R&D solution priorities identified at the 2015 DOE Materials for Harsh Service Conditions Workshop include:

- *Improved modeling and simulation* to enable better prediction of how new materials will behave in the operating environment (with regards to materials performance, stability and lifetime)
- *Smarter design of materials* with improved functional performance that incorporates predictive modeling (based on probabilistic methods) and high-throughput characterization
- *Accelerated materials qualification*, including in-situ, real-time characterization techniques for monitoring and process control of the manufacturing of materials for HSC

- Improvement of development of *advanced manufacturing techniques* to ensure that the superior properties of an advanced material are not lost when it is integrated into a fabricated component
- Match new materials with practical applications

The objective for Materials for Harsh Service Conditions identified in AMO's Multiyear Program Plan (MYPP)⁴ is to lower energy use and emissions by advancing technologies that increase durability and reduce the cost of materials and components operating in harsh and extreme environments. Identified specific technical challenges and barriers include:

- Pathway to cost-effective manufacturing
- Fundamental understanding of extreme and complex conditions
- Accelerated material discovery related to surfaces and bulk structures
- Materials for emerging harsh service conditions in flexible and advanced energy environments

Specific R&D needs highlighted in a 2019 National Academies study supported by the DOE and the National Science Foundation (NSF) include⁵:

- In situ methods to inform understanding of why materials fail under harsh conditions
- Modeling and simulation to inform understanding of properties of hybrid (e.g. metal-ceramic) materials
- Fabrication of hybrid materials
- Lightweight, high-strength, and high-toughness materials
- High temperature corrosion-resistant materials for ultra-supercritical fossil energy power systems
- Structural materials with superior resistance to ultra-high cycle mechanical fatigue
- Electronic materials for high temperature environments
- Computational thermodynamic tools to guide design of new materials, including alloys
- Fundamental understanding of corrosion and other degradation mechanisms
- Fundamental understanding and characterization of material property (e.g. strength, heat capacity, thermal expansion, thermal diffusivity, and electrical conductivity) at extreme temperatures

⁴ <https://www.energy.gov/eere/amo/downloads/advanced-manufacturing-office-amo-multi-year-program-plan-fiscal-years-2017>

⁵ National Academies Press, *Frontiers of Materials Research: A Decadal Survey*, 2019.

- Combined experimental research, theory, and computational modeling to explore fundamental materials behavior under extreme conditions to inform development of new generations of high-performance materials.

Finally, the Harsh Environment Materials Initiative (HEMI) was launched in FY2020 and was continued in the President's FY2021 Budget Request to Congress for the Department of Energy to meet the challenges of today and tomorrow by promoting energy independence, progressing scientific research, and protecting the Nation. Specifically, this cross-cutting activity between the Office of Fossil Energy (FE), the Office of Nuclear Energy (NE), and the Advanced Manufacturing Office (AMO) exploits synergies in materials and component manufacturing research for thermoelectric power plants.

3.2 Challenges, Barriers, and Opportunities

Service conditions are unique to a given application. The harshness of those service conditions are relative to the performance and limitations of the incumbent material. Therefore, the challenges and barriers associated with developing and fielding materials for harsh service conditions are specific to a given application with an associated set of performance/design requirements. These application/material specific challenges can generically be grouped into the following categories:

- **Operational Environment**: The quantitative characterization of the harsh service condition is required to overcome the challenges posed by the operational environment. The parameters that characterize the operational environment define the requirements (engineering, design, testing, experimental, etc.) that must be met to overcome the challenge. These requirements impact all aspects of addressing the challenge, including the qualification/certification of the solution.
- **Degradation Mechanisms**: A quantitative understanding of the synergetic effects of competing degradation mechanisms is necessary to overcome the challenges posed by the operational environment. Material degradation involves complex time dependent mechanisms that span multiple length scales. The elimination or effective mitigation of the degradation mechanisms must be accomplished to overcome the challenge. This includes predictive capabilities of material response, performance, and limitations in applicable operational environments.
- **Performance Demonstration**: The validation of performance is necessary in multiple stages of material development and deployment. Unique test facilities and methodologies are often required to characterize a materials response to harsh or extreme service conditions. These capabilities include specialized analytical equipment, in-situ characterization techniques, ability to apply representative operational

conditions at multiple scales, and advanced computational tools. There is also a need to reliably correlate accelerated test result to a representative service life.

- Manufacturing: A material must be capable of being manufactured at an industrial scale to be a viable solution. The material solution must also be cost effective. Cost effective manufacturing includes production of materials and assembly of parts which requires integration of materials in structures (joining, coating, sealing, lubrication, etc.) and consideration of the supply chain (e.g., raw material flexibility and recycling or reprocessing after end of use). Manufacturing includes the qualification/certification of the associated processes and resulting material.
- Materials Discovery: Accelerated materials discovery is needed to meet the demands for future power systems and energy intensive applications. Advances in Integrated Computational Materials Engineering (ICME) and understanding of microstructure-processing-property interdependences are needed to accelerate material discovery.
- Emerging Applications: The future will inevitably present challenges to materials when a variety of clean power sources play an important role in the grid. Beyond power generation, electrification, CO2 reduction, and fuel flexibility the future energy landscape will require machines and tools operating under new types of harsh conditions. Energy storage, including batteries, will enable balancing between energy generation and utilization. Energy storage will require materials designed for a high number of power cycles over a wide range of environmental operating conditions.

Additionally, some industrial sectors have unique challenges to adopting solutions for materials in harsh service conditions. These challenges often apply to applications effecting public health and safety and include federal regulations, requirements to comply with consensus codes and standards, international agreements, and/or inaccessibility of the incumbent component/material. Civilian nuclear power generation is an example of an industrial sector with unique challenges.

The material performance requirements in the civilian nuclear power generation industry are similar to other high reliability applications; although, the material degradation mechanisms are complicated by high-energy neutron irradiation. A unique aspect of a nuclear power station is that its systems/components are classified into regulated and nonregulated subgroups, depending on their intended function and if they are safety-related. The regulated components (and the materials used to fabricate them) must comply with the requirements set forth in the Code of Federal Regulation (CFR). Demonstrating compliance with the applicable requirements often entails layers of technical assurance and certifications/qualifications which typically take multiple years. Recognizing and understanding challenges of this nature are critical in successfully developing and fielding materials for these harsh service environments. The failure

to proactively address these additional requirements will substantially delay the adoption of a material solution.

3.3 Opportunities and Key Technologies or Science Areas

The Materials for Harsh Service Conditions area is complex, with multiple dimensions. These include the characterization of service conditions (generic or based on application), material class, degradation mechanisms, and solution technologies or applications. In addition, tailoring properties to meet the requirements of harsh service conditions benefit from advanced computational techniques for material discovery as well as strategies to vary composition and/or structure to enhance properties.

The Quadrennial Technology Review (QTR)⁶ identified a number of linked application areas and service conditions, and AMO's work over the past several years has focused on two of the applications: 1) high temperature materials for gas and steam turbines and 2) materials for waste heat recovery in harsh environments (including manufacturing facilities).

In the FY20 Congressional Budget Request⁷, the Administration proposed the Harsh Environments Materials Initiative (HEMI), a cross-cutting effort coordinated with Fossil Energy and Nuclear Energy to exploit synergies in materials and component manufacturing R&D for advanced thermoelectric power plants. Specifically, AMO was directed to focus on advanced materials to facilitate innovative configurations not currently possible including novel component geometries, materials that vary in composition and structure gradually over volume, sensing capabilities integrated into materials, and materials for harsh service conditions.

The FY20 senate appropriations language⁸ recommended the Manufacturing Demonstration Facility develop additive systems and automation technologies that have the potential to deposit multiple materials allowing for hybrid material solutions that enhance performance in extreme environments and enable precise property profiles. The Committee also recognized the value silicon carbide matrix composites for high temperature applications and recommended development and industrialization of a low-cost polymer infiltration process for the fabrication of silicon carbide components. The Committee encouraged the Department to

⁶ QTR 2015 Materials for Harsh Service Conditions: Technology Assessment.

<http://energy.gov/sites/prod/files/2015/02/f19/QTR%20Ch8%20-%20Materials%20for%20Harsh%20Service%20Conditions%20TA%20Feb-13-2015.pdf>.

⁷ Department of Energy FY2020 Congressional Budget Request, Volume 3, part 2, <https://www.energy.gov/sites/prod/files/2019/04/f61/doe-fy2020-budget-volume-3-Part-2.pdf>

⁸ Energy and Water Development Appropriations Bill, 2020, Senate, <https://www.appropriations.senate.gov/imo/media/doc/FY2020%20Energy%20and%20Water%20Development%20Appropriations%20Act,%20Report%20116-102.pdf>

leverage best practices from large-scale, high-rate commercial composite aerospace manufacturing.

The FY20 house appropriations language provided for process-informed science, design, and engineering of materials and devices in harsh environments, including nuclear environments⁹. This language also appeared in the house and senate conference report.

In an unpublished internal white paper, immediate application areas and service conditions were identified by AMO based on current needs, congressional direction, priorities of partner offices, and anticipated future needs:

- Materials for high pressure hydrogen storage and fueling
- Ceramic composites for high temperature applications
- Turbine applications (including asymmetric properties)
- Harsh service conditions in an electrifying manufacturing sector

Materials for Harsh Service Conditions Workshop Breakout Session Questions

For each of the six workshop breakout sessions tabulated below, several questions will be addressed:

QUESTION 1: What are the high impact opportunities for material technology and/or manufacturing process advancements in the TRL 3-6 range in energy production or energy-intensive applications involving harsh environments?

QUESTION 2: For those high impact opportunities listed above, what are the current operational and/or performance metrics, and what advancement or improvements are envisioned/targeted if a research goal is met? Please provide answers in specific terms such as temperature improvements, service life improvement, or other achievable and measurable specific performance terms.

QUESTION 3: What are the challenges & barriers that need to be overcome regardless of whether they are derived from technical issues, fabrication/manufacturing issues, market issues, supply chain issues, or material issues?

QUESTION 4: For each technology subtopic discussed in the session, what are the research and development (R&D) needs of the end-use applications and manufacturing processes? I.e., what does the OEM say they need to realize the targeted improvement?

⁹ ENERGY AND WATER DEVELOPMENT AND RELATED AGENCIES APPROPRIATIONS BILL, 2020, House of Representatives, <https://docs.house.gov/meetings/AP/AP00/20190521/109534/HMKP-116-AP00-20190521-SD003.pdf>.

Day 3 (Thursday, October 29, 2020)

11:00 am to 3:00 pm	<p>BREAKOUT SESSION #1: Materials for Extreme Temperatures, Thermal Management, and Energy Conversion (4 hrs.)</p> <p><i>Session Leads: Dr. Jeff Hawk (NETL), Dr. Kashif Nawaz, (ORNL)</i></p>
11:00 am to 3:00 pm	<p>BREAKOUT SESSION #2: Wear, Oxidation, and Corrosion-Resistant Alloys, Components, and Coatings for Static and Rotary Applications (4 hrs.)</p> <p><i>Session Leads: Dr. Bruce Pint (ORNL), Prof. Brian Gleeson (University of Pittsburgh)</i></p>
11:00 am to 3:00 pm	<p>BREAKOUT SESSION #3: Ceramics, Composites, and Functionally Graded Materials for Harsh Environments (4 hrs.)</p> <p><i>Session Leads: Dr. Edgar Lara Curzio (ORNL), Prof. Elizabeth Opila (University of Virginia)</i></p>

Day 4 (Friday, October 30, 2020)

11:00 am to 3:00 pm	<p>BREAKOUT SESSION #4: Enabling Materials through Advanced Manufacturing Technologies (4 hrs.).</p> <p><i>Session Leads: Dr. Gary Rozak (HC Starck), Dr. Isabella Van Rooyen (INL)</i></p>
11:00 am to 3:00 pm	<p>BREAKOUT SESSION #5: Accelerating Qualification of Advanced Materials & Experimental Validation of ModSim Methodology for Materials, Manufacturing, and Performance During Service (4 hrs.).</p> <p><i>Session Leads: Dr. Dave Alman (NETL), Dr. Michael McMurtrey (INL)</i></p>

**11:00 am to
3:00 pm**

BREAKOUT SESSION #6 ROUND TABLE: Mechanisms for collaborative demonstration of processes at industrially relevant scale (4 hrs.).

Session Leads: Dr. Briggs White (NETL), Dr. Rob O'Brien (INL)