Rapid Design, Development and Deployment of Materials for Extreme Environments

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ABSTRACT

The availability of low cost, durable metal alloys is a foundational requirement for achieving many of the Nation's targets for affordable, efficient power production. This need for high-performance alloys is particularly manifest as an enabler for advanced fossil energy power cycles, where extreme temperatures and/or pressures are required to maximize cycle efficiencies. The Department of Energy – Fossil Energy's (DOE-FE) program is focused on the rapid development and deployment of affordable, reliable materials that can meet the extreme demands of fossil energy power systems, utilizing an integrated materials engineering approach that incorporates computational alloy design and simulation, with best practice manufacturing, combined with focused testing and characterization to validate the alloy's long-term stability in relevant operating environments. This approach provides an efficient pathway for obtaining the desired alloy microstructure, with concomitant gains in alloy performance.

Keywords: alloys, high-performance, fossil, energy

1 INTRODUCTION

Emerging EEMs (Extreme Environment Materials) are new classes of alloys and ceramics that are not yet commercially available and will require significant research and discovery to elucidate their energy system potential, and which by their very nature may impact applications in many nascent power generation technologies. FE's EEM program provides a structured pathway for assessing the potential viability of new materials, with the goal of developing them to the point necessary for industry continue development and commercially use.

Fossil Energy EEM development focuses on identifying cost effective structural and functional materials solutions for advanced power production technologies, and in the process, reducing the cost and time needed to bring them into the energy market. Material development also explores the potential of new advanced manufacturing methods and on computational methodologies for life modeling as a cost effective enabling technology.

A major barrier to the use of new EEMs is the high cost of the constitutive elements typically used in these materials. Also, EEM manufacturing costs increase as the complexity and performance capabilities of such materials increase. For example, the cost of structural alloys for FE power plants increase exponentially as the upper use temperature and pressure of the alloys increases [1].

The DOE-FE tactical and strategic approach is to address the issues of long, costly EEM R&D development cycles and the high costs of finished products in parallel with providing necessary EEM R&D for transformational power cycles (Figure 1) that are part of the current R&D portfolio. Commercially available EEM solutions exist for state-of-the-art power generation technologies, and for many of the second-generation power generation technologies. Many materials that are suitable for use in these first- and second-generational technologies will not be suitable for next generation transformational energy systems because of higher temperatures and stresses, and more aggressive environment conditions that will exist in these newer systems. Thus, material discovery activities will remain a critical aspect of DOE-FE research in order to make the transformation jump in efficiency.

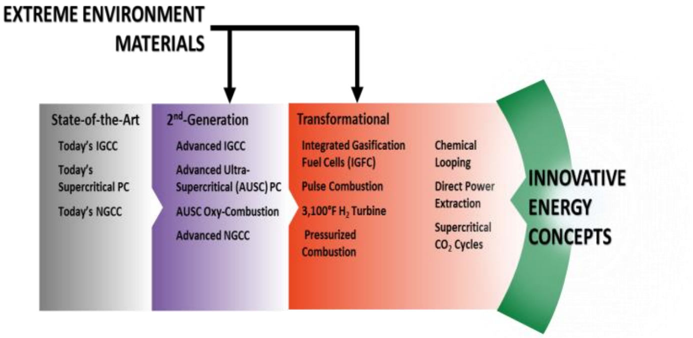

Figure 1: Fossil Energy Power Generation Technologies.

2 ADVANCED EEM MATERIALS AND CONCEPTS

Ferritic-martensitic steel, austenitic stainless steel, and nickel superalloys comprise the vast majority of the metallic materials used for structural applications in the first- and second-generation power generation technologies. The cost of EEMs increases exponentially with a linear increase in temperature capability. Also, the limit of thermal stability of commercially available nickel superalloys will be exceeded for any transformational gas turbine cycle. While ceramic matrix composites (CMCs) are being developed for some internal parts in the hottest section of a gas turbine, metal-based materials will continue to serve in high net stress applications, such as rotors, pressure tubes, piping, and casings. Thus, there are several reasons for developing even more heat-resistant EEMs that are both tough and fabricable into required component forms:

1. To replace more expensive existing alloys for the same service conditions.
2. To extend the current maximum operating ceiling (temperature, stress and corrosion/oxidation resistance) beyond the range of existing ferritic-martensitic steels, austenitic stainless steels and nickel superalloys.
3. To extend the application of existing alloys by radically improving their properties at minimal or no additional cost.

The same reasoning as that given above for development of advanced structural materials can be used to support the development of advanced functional materials, with the exception that functional materials R&D usually starts with very specific, and often single-use, application requirements (e.g., thermal barrier coatings for gas turbines or an O_2 carrier for Chemical Looping Combustion (CLC)).

Examples of materials substitution can be seen in Figure 2, which shows the maximum temperature range of ferritic-martensitic steel, austenitic stainless steel, and polycrystalline nickel superalloys as a function of design stress at a design life of 100,000 hours versus operating temperature. The chart is based on conventional melting, casting and tube fabrication methods as currently used in the industries.

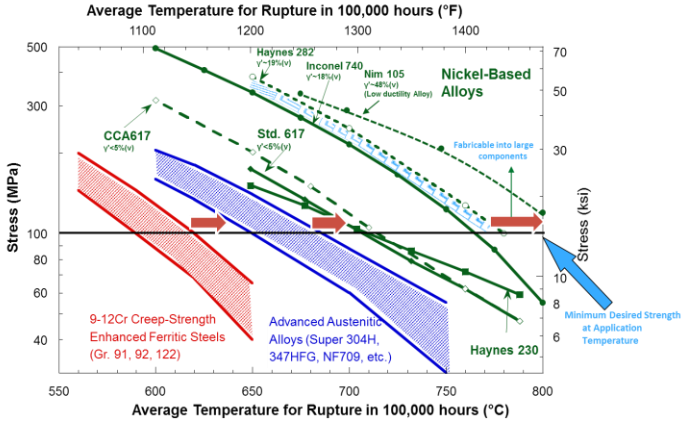

Figure 2: Increasing the Temperature Limits for 30 Year Life of Current Alloy Groups used in FE Power Generation Systems.

A reduction in EEM costs could be achieved if the maximum temperature/stress ceiling of austenitic stainless steels could be extended by about 50°C. For example, Nimonic 105 (a gamma prime precipitate strengthened polycrystalline nickel superalloy) has significantly higher creep strength than other polycrystalline nickel alloys such as Haynes 282 and Inconel 740. The cost of these three polycrystalline nickel alloys in basic ingot form is expected to be similar. Unfortunately, Nimonic 105, due to its high gamma prime volume fraction, has limited room-temperature ductility, leading to issues in fabrication of component shapes such as tube and pipe. Improved ductility of Nimonic 105 at minimal, or no, additional cost may provide an alternative to Haynes 282, while at the same time increasing the useful temperature range (i.e., up to about 800°C).

A number of material-based concepts of potential value to multiple power cycles have been identified during the past several years [2,3,4]. These concepts are based on either radical improvement of the mechanical properties of existing alloys, relatively new types of alloys, or radically different methods of combining multiple EEMS into multi-functional structures. To our knowledge none of these concepts have progressed beyond the TRL 1-3 stage.

In the discovery process whereby new alloys are envisioned, or radical modifications of existing alloys are attempted, the current approach is to first conduct an in-depth assessment (including Data Analytics if sufficient information exists) of the current state of knowledge on each concept, determining, if possible, the potential best fit for the concept within the materials hierarchy. If the initial assessment shows EEM potential, then any major manufacturing cost barriers would be explored that might limit commercialization. In any event, at the earliest possible time, computational and experimental R&D should be used to establish if the target performance properties are achievable. As an example, the very large body of computational analysis, in conjunction with experimental research [4,7,8] indicates that high entropy alloys should be further explored, especially in conjunction with Advanced Manufacturing. Research by NETL [5,6] supports this assessment. As such, this alloy “family” should be given a high priority so that the limits of its potential use as a structural alloy can be determined. Additionally, the basic high entropy approach can be applied to existing alloys in use in FE energy systems to optimize their stability, performance and life at little or no additonal base alloy cost.

Revolutionary manufacturing approaches like additive manufacturing, need to be fully exploited through continued research and development to prduce materials with unqiue microstructures and concomitatnt properties, including multi-material/multi-functional materials concepts that can an enabler for a 70 percent combined cycle efficiency gas turbine and modular chemical and power conversion reactors and devices.

3 DATA ANALYTICS

Data Analytics may very well be a key enabler for: (1) Reducing the time and cost of R&D, (2) Reducing the time and cost of certification and qualification of new EEMs, (3) Expanding options for Advanced Manufacturing, and (4) Identifying potential new EEMs based on existing ones. Data Analytics for FE EEMs can be envisioned to include:

1. Methods, Procedures and Data Storage Architecture
2. Retrieval, Assessment and Data Storage from FE/NETL Funded Projects
3. Data Analytics on Key Classes of Metallic EEMs and Ceramics EEMs

Figure 3, shows the various steps in a well-organized and structured Data Analytics project. The complexity of a particular project will depend on the problem definition and goals, and on the types and quantities of data to be assembled and analyzed. Data on EEMs may include chemistry, manufacturing process, heat treatment, microstructure, physical and mechanical properties, as well as plant performance data, if it is available. The output of computational modeling work on the design and life prediction of EEMs (i.e., derived quantities) based on the aforementioned specific EEM information may also be used as appropriate.

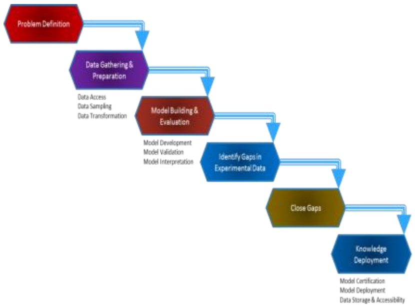

Figure3: Data Analytics Data Mining Process.

The National Institute of Standards (NIST) and DOE (e.g., in MGI) are funding a considerable amount of R&D to develop standards, procedures and methods for the storage, retrieval and assessment of materials properties data. data from these projects will be applicable to both experimental and computational generated data for a very broad range of materials. Thus, the recommended strategy for EEM Data Analytics will be able to assemble as much of the software, database architecture, and assessment methods as possible from other government organizations. This data would provide a path forward for many energy related outcomes, leading to more effective use of these alloys in power cycles:

1. Identify the best architecture, software and processes for future EEM Data Analytics
2. Develop framework and procedures to be used for future EEM data analytics projects
3. Answer several important and long-unanswered questions leading to variability in mechanical behavior of 9-12 percent chrome steels.

With respect to (3), any information could significantly reduce the time and cost of certification of new alloys, provide general but more accurate models of long-term mechanical behavior, and focus future R&D in alloy melt processing and minor element control for better alloy performance.

As this effort moves forward, leading to an EEM Data Analytics framework, future work could progress on two parallel paths: Use Data Analytics process to retrieve, assess and archive the results of all completed EEM R&D projects: Apply Data Analytics approach to assess other potentially useful EEMs that might otherwise have been overlooked by applying Data Analytics to other critical EEM classes.

A major challenge in assembling data within a material class is obtaining access to data that may have been generated from many organizations for specific competitive reasons. Some of this information may be available in limited form (e.g., the National Institute for Materials Science (NIMS) online database) while for other organizations such as the European Collaborative Creep Committee (ECCC), the only data available to the public is in nominal terms and/or is derived (i.e., no specific individual data associated with specific chemistry). Additionally, much other information is company proprietary or organization sponsored. Access in these instances would have to be negotiated in some manner with the likely consequence of partner limited access to data after its use. Access may require making a financial commitment to these organizations to use the data while at the same time agreeing to withhold it from public dissemination.

Another challenge is the quality of the data used. The power of the data analytics process is supposed to be that gaps in data do not necessarily hinder analysis, but this only applies if there is sufficient data within each category that can be interrogated properly in order to assess the trends relative to the missing data. For EEMs this may be a problem in that there might not be sufficient data available such that gaps can be managed with confidence. Consequently, it may be necessary to provide specific experimental information (e.g., microstructure and mechanical properties or selected experiments) to fill these gaps for more effective analysis.

4 COMPUTATIONAL MODELING OF LONG-TERM BEHAVIOR OF MATERIALS

DOE FE/NETL's modeling expertise and experimental data bases now exist to develop and validate physics-based constitutive creep equations for a range of polycrystalline nickel superalloys that are of interest to both DOE-FE and NE. FE/NETL R&D projects on AUSC materials have resulted in creep data on Inconel 617, Inconel 740, Haynes 282 and Nimonic 105 that extend past 20,000 hours and up to about 100,000 hours for some alloys. In parallel, DOE-Office of Nuclear Energy has generated creep data on Inconel 617 at the conditions expected in the next-generation nuclear reactor. (These conditions involve higher temperatures and lower loads than a FE AUSC power plant.) FE-NETL projects have demonstrated that a single physics-based equation can describe, accurately, the creep behavior of Inconel 740, Haynes 282 and Nimonic 105 (with material constants adjusted for each alloy). It is anticipated that with some modification the same model can describe the creep behavior of Inconel 617. Thus, the creep behavior of a broad range of solution and precipitate strengthened polycrystalline nickel superalloys (from a few volume percent precipitates to about 45% precipitates) can be described by a single generalized creep equation. This approach will also be capable of describing the creep behavior of other polycrystalline nickel superalloys. The constitutive creep models developed for each alloy will provide two major benefits:

1. They will support the cases for component design by analysis, reducing alloy certification requirements.
2. They will improve the accuracy of Finite Element (FEM) based design of components made from these alloys, resulting in more efficient component designs.

While creep is an important deformation process, most components undergo creep-fatigue. Once the creep model have been developed and verified, a similar effort would develop a combined creep and creep-fatigue framework. A suitable alloy system would need to be identified that had sufficient creep, fatigue, and some creep-fatigue data (although this could be produced in the laboratory for specific conditions). Several candidate systems are possible, including Inconel 617, Haynes 282, and Inconel 263, possibly 316 SS, and a ferritic-martensitic alloy like P91.

5 CONCLUSION

The primary motivations for the DOE-FE effort are: (1) EEMs are often key enablers for successful development of advanced, efficient and economically competitive power cycles; (2) advanced power cycles usually require EEMs with performance capabilities beyond those of existing commercially available materials; and (3) development and commercialization of new EEMs is a long, expensive and high risk process, especially for FE energy systems where design life of a structural EEM is on the order of 10 to 40 years.

Commercial EEMs are available for state-of-the-art FE power generation technologies, and for many of the FE second-generation energy systems. Many materials that are suitable for use in first- and second-generational technologies might not be suitable for future transformational power generation technologies because of higher temperatures, higher pressures, higher stresses, and/or more corrosive conditions that will exist in these systems. Thus, material design and discovery activities remain a critical aspect of transformational and visionary DOE-FE research.

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