ReNeW White Paper: Major Materials Issues for DEMO

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Introduction

Overcoming the materials and structures challenges for first-wall, blanket and diverter systems is as difficult and important for fusion energy generation as achieving a burning plasma. Fusion materials and structures must function in a uniquely hostile environment that includes various combinations of high temperatures, reactive chemical interactions, time-dependent thermal and mechanical stresses, and intense neutron fluxes. Atomic displacement damage alone in a DEMO type reactor is equivalent to ejecting every atom from it's lattice site up to 200 times. Displacement damage undergoes complex interactions with high concentrations of reactive (e.g., H) and insoluble (e.g., He) gases that leads to the degradation of a host of performance sustaining material properties, through processes such as hardening, low temperature embrittlement, phase instabilities, segregation, precipitation, irradiation creep, volumetric swelling, and high-temperature He embrittlement. Plasma facing components must also withstand severe attacks heat fluxes comparable to that experienced by rocket nozzles. At the same time, key fusion structures are subject to a wide variety of poorly understood failure paths, while they must clearly demonstrate high safety margins over long lifetimes. Indeed, the unprecedented demands placed on materials from thermomechanical loading alone are a feasibility issue, even without the severe effects of radiation damage.

Material properties depend on composition and microstructure at length scales ranging from sub nm to cm. Within limits, the microstructures of materials can be manipulated to optimize some, but usually not all, relevant properties. Thus, tailoring microstructures provides a potentially viable approach to developing radiation-resistant materials for fusion with a requisite balance of performance sustaining properties. Typically, alloys contain five or more constituents, two or more phases as well as complex dislocation and grain boundary defect structures. The detailed morphology and distribution of these features control properties. Like a burning plasma, useful microstructures are almost always in a far from equilibrium thermodynamic state that evolves with time. Radiation damage further drives microstructural evolution, including the formation of new features and micro and macro damage. Creating and sustaining optimal microstructures is a scientific grand challenge that must also deal with practical complexities of fabrication, including processes such as welding. Thus design of alloys or composite architectures for sustained performance of severely challenged fusion structures will require a highly disciplined, long term effort that is based on cutting edge science. While we focus on metallic alloys, it should be noted that many of the same technical challenges must also be addressed for composites, functional, and special purpose materials.

The fusion materials sciences program is focused on determining the underlying physical mechanisms controlling the performance of materials in the harsh fusion environment. It is well established such a science-based approach is the most efficient path for developing materials for challenging environments. For example, a worldwide effort involving hundreds of scientists over a period of 20 years overcame several major technical hurdles to successfully develop Ni_3Al intermetallic high-temperature alloys with sufficient ductility and fabricability for commercial applications in 2003 (initial products are furnace fixtures and rollers used for steel fabrication; higher performance structural applications will presumably follow once sufficient industrial experience is obtained). Similarly, a dedicated science-based 14 year, 175 M$ effort recently developed four successfully improved generations of Si_3N_4 ceramics with a resultant four-fold increase in high-temperature strength that enabled monolithic ceramics to become reliable structural materials for certain low-stress applications. The historical precedent for development of structural materials ranging from aircraft turbine components to pressure vessel materials is that a period of 10-20 years with 150-200 M$ budgets are required for successful development. However, the development challenges for these materials systems pale by comparison to that for fusion materials, which is arguably the greatest materials development challenge in history. The combination of high temperatures, high radiation damage levels, intense production of transmutant elements (in particular, H and He), high thermo-mechanical loads that produce significant primary and secondary stresses, and time dependent strains for which no high-temperature design codes exist requires very high performance materials for fusion energy systems.

Major Scientific and Technical Challenges

Helium Effects

A unique aspect of the DT fusion environment is the production of very large quantities gaseous transmutation products such as He and H - at 200 dpa approximately 2000 appm of He and 8000 appm of H. Most of the H diffuses out, but some may be trapped at bulk defects and interfaces, enhancing such phenomena such as void nucleation and H-embrittlement. Due to its low solubility, He precipitates into clusters or gas bubbles. At high temperatures grain boundary He bubbles grow and coalesce under stress, resulting in severe degradation of creep and fatigue properties. In austenitic stainless steels the creep rupture life was lowered by about two orders of magnitude by introduction of 200 appm He in the microstructure. At lower temperatures there is growing evidence that high He synergistically interacts with hardening, resulting in severe degradation of toughness and intergranular fracture. Ductile-to-brittle transition temperature shifts as large as 700°C have been measured in spallation proton irradiations of reduced activation ferritic/martensitic (RAF/M) steels, which renders such steels unusable in the fusion environment. At intermediate temperatures He bubbles may serve as nucleation sites for growing voids, potentially leading to swelling and enhanced creep rates. Thus there may be a very limited window of for RAF/M steels in first wall and blanket structures.

Fission reactor environments generally do not produce high quantities of He in RAF/M steels. However, the effects of high He levels have been studied in mixed spectrum reactor irradiation experiments by doping with elements like Ni and B which have large thermal neutron (n,α) cross sections. Some of these studies have also involved combinations of neutron spectral and alloy isotope tailoring. Unfortunately, interpretations of doping studies have generally been severely confounded by a number of factors. Alloys can isotopically enriched in ^{54}Fe to enhance He production, but this is very expensive and produces He at a rate lower than in a fusion spectrum. Likewise dual ion irradiations can provide useful information on the mechanisms of displacement damage-He synergisms, but cannot simulate the fusion environment due to effects of their highly accelerated dose rates and limited ranges of the charged particles. Irradiations in spallation proton beams produce He/dpa ratios that are higher than for fusion, but have been beset by temperature control issues. Recently, an innovative approach to mitigating some of the limitations noted above has been implemented based on *in-situ* He implantation of Ni bearing injectors at fusion relevant conditions. Preliminary results from this research shows that He bubbles decorate the boundaries of RAF/M steels and that matrix He bubbles are the nucleation sites for voids. The observations suggest that RAF/M steels will be vulnerable to the various forms of embrittlement and damage cited above at dpa levels far below lifetime targets. The fusion materials program will use all of these techniques, closely integrated with state of the art modeling studies, to build a knowledge base on the effect of fusion relevant irradiation effects.

However, understanding and even predicting He effects is not sufficient. New alloys must be designed to manage the effects of high levels of both He and displacement damage. Indeed, the U.S. fusion materials sciences program is exploring a promising new alloy class, known as nanostuctured ferritic alloys (NFAs). NFAs contain an ultrahigh density of nm-scale non-equilibrium Y-Ti-O enriched phases (NFs) that may give unprecedented high-temperature creep strength, radiation damage resistance, and efficient trapping of He. Preliminary in situ helium implanter data suggests that the NFs suppress void swelling and protect GBs from He accumulation. While these materials are in their infancy, they offer great promise for fusion applications. Ultimately, the irradiation performance of RAF/M steels and NFAs must be verified by high-dose neutron irradiations. The facilities that will be needed to perform such research are described below.

High-Temperature Deformation

As noted in the introduction, the problems of radiation damage may only exacerbate the otherwise unprecedented challenges posed by the severe time-dependent thermal-mechanical high temperature loading of very large and complex fusion structures. A great scientific challenge is to develop physical models of high-temperature creep and creep-fatigue interactions. Current treatments of these phenomena are largely empirical and material condition specific. High-temperature design rules evolved from a body of structural application experience that is enormously less complex than in the case of fusion.

Creep models must simultaneously treat the evolutions of complex dislocation, interface and precipitate structures, stress driven dislocation climb and glide, the interaction of dislocations with obstacles, grain boundary sliding and diffusion creep that accounts for the multiple effects of grain boundary precipitates. While the effects of displacement damage accumulation diminish with increasing temperature, evidence is mounting of interactions between radiation defects with thermally induced microstructural instabilities that both accelerate and broaden the temperature regime processes that can lead to severe reductions in the strength of RAF/M steels. Helium may also influence creep rates and microstructural instabilities. However, again, the major effect of He is to greatly enhance creep cavitation, thus severely reducing creep rupture life.

The effects of cyclic plastic loading are far more damaging than for monotonic loading, especially in regimes with long tensile hold times, or when creep cracks develop. While outstanding work has been carried out on high-temperature properties in the past, this area of research has basically lain dormant for the past 20 years. However, given the wide array of new experimental, computational and modeling tools available today, there is a tremendous opportunity and, indeed, imperative to develop new models of high-temperature deformation and fracture phenomena tailored to fusion materials, including thermal-mechanical-irradiation synergisms. These models are needed to guide development of stable, creep and damage resistant alloys, like NFAs.

Corrosion, Compatibility and Coatings

Corrosion and compatibility may also limit first-wall and blanket upper temperature limits. Chemical interactions of coolants, breeder materials and structural alloys involve multiscale-multiphysics phenomena. The traditional approach to study corrosion has been almost entirely empirical, based on static coupon testing and flowing coolant in a temperature gradient. However, empirical correlations of corrosion rate to coolant temperature and flow velocity do not capture the fundamental physical mechanisms involved and, therefore, do not provide predictive capability outside the range of the experimental measurements. Thus a significant opportunity exists to improve the scientific understanding of corrosion through controlled experiments combined with physical models based on advanced computational thermodynamics and kinetics codes. These models can be used to design integrated flow experiments that can also be greatly enhanced by use of sophisticated *in situ* diagnostic and sensor technologies. Corrosion and compatibility are also closely linked with thermal-mechanical conditions, like environmentally assisted cracking, but these issues have not yet been addressed for fusion materials and conditions. A parallel effort to develop of a science-based approach to coatings for fusion applications also presents a great opportunity.

Low-Temperature Deformation & Fracture

The low-temperature operating limit for most fusion structural materials is dictated by radiation hardening and helium embrittlement, manifested as severe fracture toughness degradation and decreased uniform tensile ductility to less than 1%, even at very low fluence. Like other types of radiation damage, embrittlement depends on the synergistic combination of many environmental and material variables. Thus, multiscale models are needed to predict the evolution of these properties. While major progress has been made in recent years, the ultimate objective of fully basing such models on predictions of microstructural evolution will require a sustained effort and a high quality database, including at high dpa and He/dpa ratios. Our strategy is to relate microstructural evolutions to changes in basic structure sensitive properties, that are then used to model more complex engineering properties, like fracture toughness, including at the component scale. The latter is important step, since both measurement and application of material 'properties' often depends on the specimen–structure geometry.

Towards this end, a master-curve-shifts method has been developed by the fusion materials program, that represents an enormous advance in predicting fast fracture limits of embrittled structures. However, issues related to the existence and physical basis for an invariant shape of the master curve, effects of shallow cracks and, especially, the embrittling synergisms between hardening and He all remain to be resolved. Similarly, the causes and consequences of complete loss of uniform ductility are not understood and involve combinations of very complex flow instabilities and localization at many length scales.

We also note that low-temperature irradiation creep is a very important phenomenon leading to inherent dimensional instabilities in fusion structures. The detailed mechanisms and variables that control irradiation creep and concomitant damage are not fully understood. Again models of embrittlement, ductility exhaustion and irradiation creep will be needed to guide the development of higher performance materials.

Theory and Modeling

The need to perform irradiation experiments cannot be replaced by modeling alone. Conversely, a purely experimental approach to understanding the effects of irradiation service on material behavior is also not practical. The cost to design, perform and examine materials from reactor irradiation experiments is high. Further, there is a combinatorial problem in that the broad range of materials, phenomena, and irradiation variables, and variable combinations, makes a purely experimental approach intractable. Robust computational models provide a means to re-evaluate existing data, optimize the design and execution of new experiments, and interpret the results from those experiments. The ultimate goal is to use validated models to improve existing materials or to design better materials. Physically based multiscale models describing irradiation and mechanical damage processes for fusion applications are still under development. Numerous fundamental details such as the migration behavior of small point defect clusters are not yet resolved. Models of key properties that simultaneously span length and time scales ranging from atomistic to the continuum and from sub-picosecond to years are needed. The following is a brief summary what needs to be developed to accomplish this goal:

- Computationally efficient and physically robust interatomic alloy potentials, including directional bonding and magnetism (to accurately describe complex multi-component, multi-phase materials).
- Advanced large-scale, atomistic models that describe the very large number of material parameters and processes that interact in complex ways to control the migration, interaction, and accumulation of defects and gases, as well as the non-equilibrium rearrangements of solute constituents by segregation and phase transitions (to predict nano-scale evolutions in complex materials for both processing and extended service).
- Linked atomistic, mesoscopic, and continuum deformation and fracture models (to predict hardening, plastic instabilities, transitions from ductile-to-brittle and creep/creep rupture behavior for complex materials and loading conditions).
- Large-scale structural models that integrate all degradation phenomena (needed for virtual integrated testing and materials-component development).

Safety and Environmental Attractiveness

A key challenge is development of high-performance materials that provide for an economically attractive fusion power system while simultaneously achieving safety and environmental acceptability goals. Radioactive isotope inventory, and release paths are important considerations in designing for safety. Development of low or reduced activation materials is central to ensuring that structural materials removed from service will not require long-term geological disposal and may offer the potential for recycling, thus further minimizing impact on the environment.

Critical Facility Needs

Irradiation experiments provide an opportunity to systematically investigate single-variable or synergistic multiple-variable effects on materials under conditions approaching the DT fusion environment. At present, fission reactors are the primary means of investigating the effects of irradiation on fusion materials. Ongoing fundamental studies have established that the key atomic displacement features for DT fusion neutrons interacting with materials are similar to those found with fission neutrons. This validates much of the fission test reactor database as a valuable initial screening tool for identifying candidate materials, and, along with other experimental tools and models, exploring key phenomena. Significant resources are required for the design and fabrication of specialized assemblies for irradiation of test specimens and for operation of hot cell facilities for disassembly of experiments and remote testing of the irradiated specimens. Techniques such as tailoring of the neutron energy spectrum, or tailoring the isotopic composition of the alloy to control transmutation rates are used to more nearly reproduce the fusion environment. *In situ* He implantation studies and spallation proton irradiations will also be useful. In addition, specialized studies using ion beams can be conducted. However, the response of materials to these various radiation fields can be quite different from that which is due to a fusion neutron spectrum and a high energy MeV neutron source is needed to develop and qualify fusion materials. A suitable neutron source must reproduce the key attributes of the fusion spectrum, particularly in terms of the He/dpa ratio. In addition, the neutron source must have flux and fluence capabilities that are sufficient to allow accelerated testing to end-of-lifetime doses. International assessments have concluded that the basic requirements for this facility include: $\geq$0.5 liter volume with $\geq$2 MW/m^2 equivalent 14 MeV neutron flux to enable accelerated testing up to at least 10 MW yr/m^2 (with larger volumes at lower neutron fluences), availability $\geq$70%, and flux gradients $\leq$20%/cm.

Ultimately, a dedicated facility to enable system level component testing, such as blanket modules, is needed to explore the potential for synergistic effects and failure paths that are not revealed in controlled material property studies. Integral tests of this type help to validate models of materials and structural performance and provide insight on possible synergistic phenomena that could compromise system reliability and performance. Such experiments must be fully informed by the property models derived from the separate-effects studies in a prototypic fusion environment and structural models validated by semi-scale type experiments.