Advanced Material Design for Fusion Applications

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Technology to be assessed

Advanced applications in a great variety of fields demand materials with superior properties able to withstand the extreme environments often required in such applications. The constant search for more efficient, reliable and safe energy sources requires exceptional control over the material properties during their entire operational life. Therefore, prediction and control become paramount in the quest for advanced materials. Fusion energy exemplifies one such application, requiring materials with extraordinary properties able to withstand exceptional temperature and stress gradients, radiation damage, high concentrations of transmutation products (H, He), and/or plasma exposures. The development of such materials poses many challenges that need to be addressed for fusion energy to become a viable power source.

Key components in magnetic fusion reactors, such as the divertor or the plasma-facing materials (PFMs), are required to have stringent properties including low activation, high melting point, good thermo-mechanical properties, low sputter erosion and low tritium retention/co-deposition. They must operate at high temperatures (≥ 1000 K) for long durations (> 10⁷ s), without failure or extensive erosion while exposed to large plasma heat and an intense mixture of ionized and energetic neutral species of hydrogen isotopes (D, T), He ash (fluxes > 10²⁴ m⁻²s⁻¹) and neutrons¹. Tungsten (W) is the leading PFM candidate due to its high melting temperature, low erosion rates and small tritium retention. These advantages are unfortunately coupled with very low fracture toughness characterized by brittle transgranular and intergranular failure regimes, which severely restrict the useful operating temperature window and also create a range of fabrication difficulties. Furthermore, blistering at moderate temperature (<800K) by D and He²,³ and the formation of pits, holes and bubbles by He at higher temperature (>1600K)⁴ have all been observed. The formation mechanisms that underpin these phenomena are not well understood but have largely been attributed to the accumulation of diffusing D and He in extended defects. In the slightly lower temperature range 1250-1600 K, the formation of nanometer scale bubbles is observed⁵ in W exposed to He plasma. At larger He ion fluences, close to ITER⁶ working conditions, exposed surfaces are found to exhibit a nanostructured surface morphology⁷, termed as fuzz. The increased surface area and fragility of these nanostructured surfaces raises new concerns for the use of W as a fusion reactor PFM, particularly as a source of high-Z dust that will contaminate the plasma.

Strong synergy between modeling and experimental efforts is required to overcome the challenges posed by fusion technology, both in the design and prediction of materials response to extreme environments. Multi-scale modeling will have to provide guidance to the proposed experiments and the experiments will need to inform and validate the models in a self-consistent loop to obtain the deepest possible understanding of the processes.

In the following we describe possible materials design strategies to improve the materials performance in these harsh fusion environments. All these technologies would need basic research (TRL1) to understand their response under fusion conditions and to optimize their properties via synthesis and processing.
Materials design strategies for improve performance

1. Nanostructured Tungsten

Nanostructure engineered pure W is being investigated to improve the material processing and working properties\(^9\). Related to this strategy, recent work by members of our team shows that state-of-the-art nanocrystalline W samples with grain sizes below a threshold (~35 nm) exhibit significant mitigation of bubble density, and bubble area. These materials also present a remarkable swelling resistance in the grain matrices when irradiated with 2 keV He at high temperatures. Grain boundaries were decorated with He bubbles which confirms the high He trapping behavior of nanocrystalline W\(^9\). No effect of ion dose was observed on the irradiation damage vs grain size behavior. An increased He dose threshold for fuzz formation was also observed on these samples\(^9\).

2. Refractory Low-Activation High Entropy Alloys

High-entropy alloys (HEAs) have been recently proposed as structural materials in a variety of applications, from advanced nuclear reactors to superconductive materials\(11-14\). These alloys are based on equiatomic compositions of several principal elements\(11,14,15\). The configurational entropy of mixing in multicomponent alloys tends to stabilize the solid solution based on simple underlying face-centered cubic (fcc) or body-centered cubic (bcc) crystal structures. Equiatomic compositions maximize this entropic term, promoting random solutions versus intermetallic phases or phase decomposition. The intermetallic phases might be desirable for certain applications but in general reduce the material ductility, and, therefore, they are typically inadequate for structural operation. Some of the HEAs show superior mechanical properties to traditional materials, which in general link to dislocation features. These materials can display high hardness values, high yielding strengths, large ductility, excellent fatigue resistance and good fracture toughness. W-based refractory HEAs have been recently developed in the context of high temperature applications, showing high melting temperature (above 2873 K) and superior mechanical properties at high temperatures compared to Ni-based superalloys and nano-crystalline W\(^9\) samples\(16,17\). The severe lattice distortion present in these alloys leads to sluggish diffusion, which improves the thermal creep resistance. We hypothesize that the response of these alloys upon He exposure and implantation will be superior to traditional alloys, due to He trapping at
tensile sites, reducing He mobility and thus decreasing the probability for bubble formation. That is, we expect the inherent slower diffusion exhibited in such alloys\textsuperscript{12,14} to lead to smaller, more dispersed bubbles that are less detrimental to performance. The effect of He is indeed unknown as no study is available in the literature devoted to the behavior of He and its coupling with the mechanical properties in these material systems. The studies of thermal conductivity and tritium retention are also essential and will have to be investigated in detail. To develop this technology would be crucial to understand the relation between composition and properties such as melting temperature, entropy of mixing and lattice distortion.

Recently, our group has synthesized single phase WTaCrV HEA films with thickness of 2.5 μm (as presented in Fig. 2). The target was to deposit an equiaxial composition thin film. The Energy Dispersive Spectroscopy (EDS) analysis indicates slight W and Ta enrichment in the film, which can be definitely adjusted by tuning the correlated deposition power. On the other hand, the EDS mapping on both surface and cross-sectional areas, and X-Ray Diffraction (XRD) results show a single bcc phase uniformly distributed. This result demonstrates our ability to deposit uniform single-phase HEA films with tunable chemical composition. Nanoindentation tests were performed, showing hardness of the film on the order ~15 GPa, which can be compared to ~9 GPa of unirradiated nanocrystalline W.

3. W-Based Additive Manufacturing Microstructures

Additive manufacturing (AM) is a synthesis process for making 3D solids of virtually any shape from a digital model\textsuperscript{19–24}. AM is distinct from traditional subtractive machining techniques, which rely on removal (as opposed to addition) of material by methods such as cutting or milling. Metal AM techniques can deliver parts with complex geometries, minimal waste material, and limited post-processing. The spectrum of available metal-powder materials provides the opportunity to fabricate parts for a wide range of applications, including aerospace, nuclear power, and ground transportation. However, AM microstructures can vary considerably from those produced by traditional metallurgical processing. It is essential to characterize and control the microstructure and properties of AM parts such that they may be qualified for use in critical applications. Furthermore, understanding how build parameters affect the microstructure will enable functionally graded materials\textsuperscript{25}. The two main technologies developed for metal processing are powder bed fusion (PBF) and direct energy deposition (DED). Both predominantly use lasers as heat sources. AM is characterized by extremely high heating and cooling rates (10\textsuperscript{3}–10\textsuperscript{6} °C/s) and temperature gradients (≥1000 °C/cm).

\begin{figure}
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\includegraphics[width=\textwidth]{image1.png}
\caption{(Top) A SEM image of the deposited WTaCrV HEA film. The correlated EDS mapping shows that the four elements are homogenously distributed. (Bottom-left) TEM micrograph with corresponding diffraction pattern resulting in strong (110) texture and half-micron grain sizes. (Bottom-right) XRD profile of the WTaCrV film, indicating a single bcc phase.}
\end{figure}

\begin{figure}
\centering
\includegraphics[width=\textwidth]{image2.png}
\caption{Microstructure of a) traditional wrought 316L steel and b) AM synthesized 316L steel showing lacy ferrite solidification structure not found in microstructures manufactured using standard wrought processing\textsuperscript{2018}.}
\end{figure}
K/s), well above traditional technologies. At these high rates, the materials system is significantly out of equilibrium, with large thermal gradients and rapidly moving solid-liquid interfaces that produce thermodynamic forces driving intrinsic defects (vacancies and self-interstitials), impurities and solute elements towards aggregation, dissolution or segregation to interfaces. The extreme heating/cooling rates lead to physical and mechanical properties substantially different from their conventionally fabricated counterparts\(^{18}\). As an example, Fig. 3 shows 316L stainless steel fabricated via a) traditional wrought processes and b) DED AM at LANL. The latter displays a novel microstructure with metastable phases and precipitates. One key condition for a material to be suitable for severe irradiation applications is its microstructural stability. In the case of the AM 316L shown in Fig. 3b, the metastable phases persisted after conventional post-fabrication heat treatments. One of our hypotheses is that the structure is constrained in a deep metastable free energy minimum, which confers substantial stability to the material. If this stability were transferable to harsh irradiation environments, the high density of microstructural features acting as defect sinks would increase the radiation tolerance of the material.

A large number of parameters, acting at the synthesis stage, control the final microstructure, including laser energy, pulse duration and penetration, heat transport properties of the material, number of laser passes, and material composition. Rather than exploring this multidimensional space via an Edisionian trial and error approach, modeling and experiments should be integrated to first understand and then predict and control the AM microstructures. This understanding will allow us to generate microstructures, both surface and bulk, ideally suited for fusion environments in an unprecedented manner.

One of the most challenging issues for structural materials in fusion energy systems involves the accommodation of intense heat fluxes while maintaining mechanical and structural integrity during exposure to high doses of energetic neutrons and He particles. In some cases, further advances in high heat flux capability are limited by the inability to precisely fabricate intricate cooling channel geometries into components using conventional machining techniques. AM might be a manufacturing route to design and build W-based PFM with geometries that optimize the heat transfer properties and the radiation tolerance.

4. Oxide Dispersion Strengthened Ferritic Alloys

Oxide dispersion strengthened ferritic alloys with small grain size (e.g. nanostructured ferritic alloys) show great promise for these demanding applications. These materials are ferritic alloys with high chrome (9-14Cr) with a high density (>10\(^{23}/\text{m}^3\)), fine distribution of nanosized (~2 nm) oxide particles and a fine grain size (<0.5 \(\mu\text{m}\)). This fine microstructure provides the alloy with high strength at high temperatures and excellent radiation tolerance (e.g. reduced void swelling and retain ductility at low temperatures; and the oxide particles help manage the helium particles generated from nuclear reactions). Recently, a large heat of 14YWT was produced (>50 kg) and testing of these materials is underway\(^{26,27}\). These materials show excellent radiation tolerance from ion irradiations to doses up to 585 dpa\(^{28}\). Additional research is needed for producing these alloys, testing the properties as well as processing into engineering forms.
Citations


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