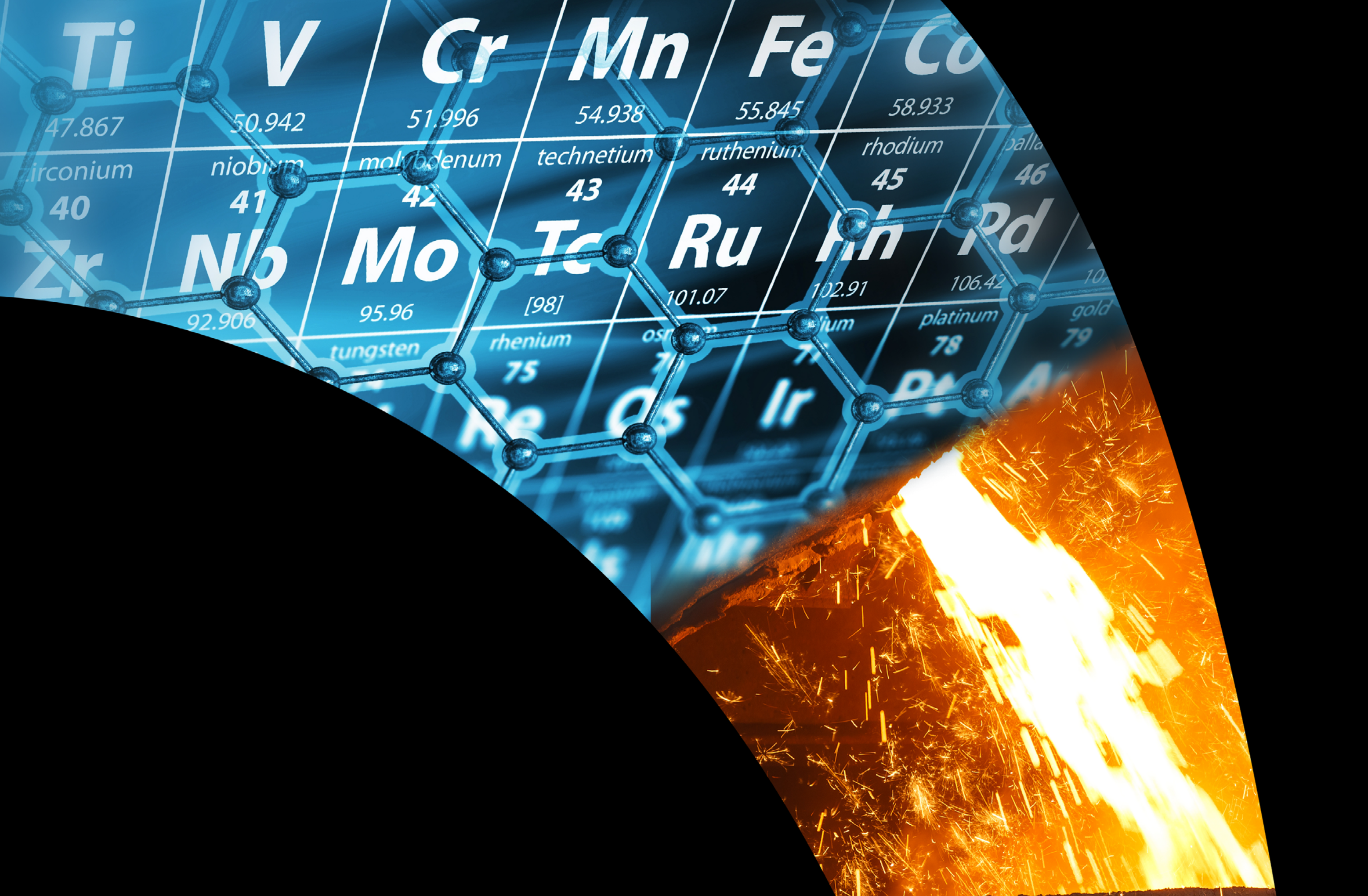

MANUFACTURING HIGH ENTROPY ALLOYS

Pathway to Industrial Competitiveness

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Manufacturing High Entropy Alloys

Pathway to Industrial Competitiveness

September 2018

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MForesight: Alliance for Manufacturing Foresight serves as the voice of the national advanced manufacturing community, providing government, academia, and industry with information and analyses about emerging technologies, workforce training, and opportunities for public-private partnerships that strengthen U.S. competitiveness.

This material is based upon work supported by the National Institute of Standards and Technology and the National Science Foundation under Grant No. 1552534 through a cooperative agreement with the University of Michigan (PI: Prof. Sridhar Kota). Any opinions, findings, conclusions, or recommendations expressed in this material are those of MForesight and do not necessarily reflect the views of the National Institute of Standards and Technology, the National Science Foundation, or the University of Michigan.

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Executive Summary

High entropy alloys (HEAs) provide a transformative opportunity to design materials that are custom tailored to the distinct needs of a given application, thereby shifting the paradigm from "apply the material you have" to "engineer the material you need." HEAs will enable high-performance manufactured goods that are competitive in the international marketplace through extraordinary material properties and unique property combinations. HEAs deliver new choices to manufacturers to create alternatives to materials that are rare, hazardous, expensive, or subject to international restrictions or conflict.

The potential benefits of HEAs span diverse fields and applications, and show promise to not only accelerate economic growth and domestic competitive advantage, but also address pressing societal challenges. These include solid state cooling, liquefied natural gas handling, nuclear degradation-resistant materials, corrosion-resistant heat exchangers, and efficiency gains from high temperature performance that advance national energy goals; high-performance aerospace materials and ultra-hardness ballistics that support national security; and strong, corrosion-resistant medical devices and advances in magnetic resonance imaging that are essential to national health priorities. Research advances are setting the stage to realize each of these vital areas.

However, research advances made to-date to produce lab-scale prototypes do not lend themselves to manufacturing at scale. For Americans to fully benefit from HEAs, the emerging technologies must be translated into products manufactured at scale in the United States. However, manufacturers and HEA experts who are working to bridge this gap are encountering cross-cutting barriers in manufacturing processes, testing, data, and access to the necessary resources. Through strategic public- and private-sector research and investment, these barriers can be overcome.

The United States has invested in both HEA research and advanced materials resources, such as material sample creation at the Ames Laboratory Materials Preparation Center, material characterization at Oak Ridge National Laboratory's Neutron User Facilities, and modeling and analysis through the National Institute of Standards and Technology's Material Genome Initiative. A vast array of research and expertise has been fostered at federal laboratories and universities, yielding promising alloys, manufacturing processes, and analysis methods.

MForesight: Alliance for Manufacturing Foresight convened leading U.S. industry, research, and government experts and practitioners to gather insights and identify the cross-cutting prospects and challenges for manufacturing HEAs in the United States. In line with its mission to coordinate input from the manufacturing community to inform national priorities in advanced manufacturing, MForesight has distilled four actionable recommendations aimed at advancing U.S. competitiveness in HEA manufacturing:

- **Invest in critical translational research for HEA manufacturing,** from the earliest alloy identification to processes enabling final part production. HEA processing technologies need to be developed past the prototype stage to enable scalable manufacturing.
- **Establish a National Testing Center for HEAs** focused on high-throughput testing to enable rapid discovery, testing, and validation of HEAs and manufacturing processes.

- **Develop a central database for HEA data** to minimize duplicative efforts and to accelerate innovations by U.S. researchers and manufacturers.
- **Enhance collaborative efforts** through increased access to federal facilities and expertise and the establishment of an interdisciplinary working group. Leveraging and alignment of existing federal resources and efforts will be essential to these efforts.

By manufacturing HEAs at scale, the United States can seize important opportunities across a range of fields, boosting economic competitiveness, and advancing national interests from defense to energy to health care. These recommendations represent a practical roadmap to realizing these goals. The technical details for each recommendation are summarized below.

Technical Recommendations

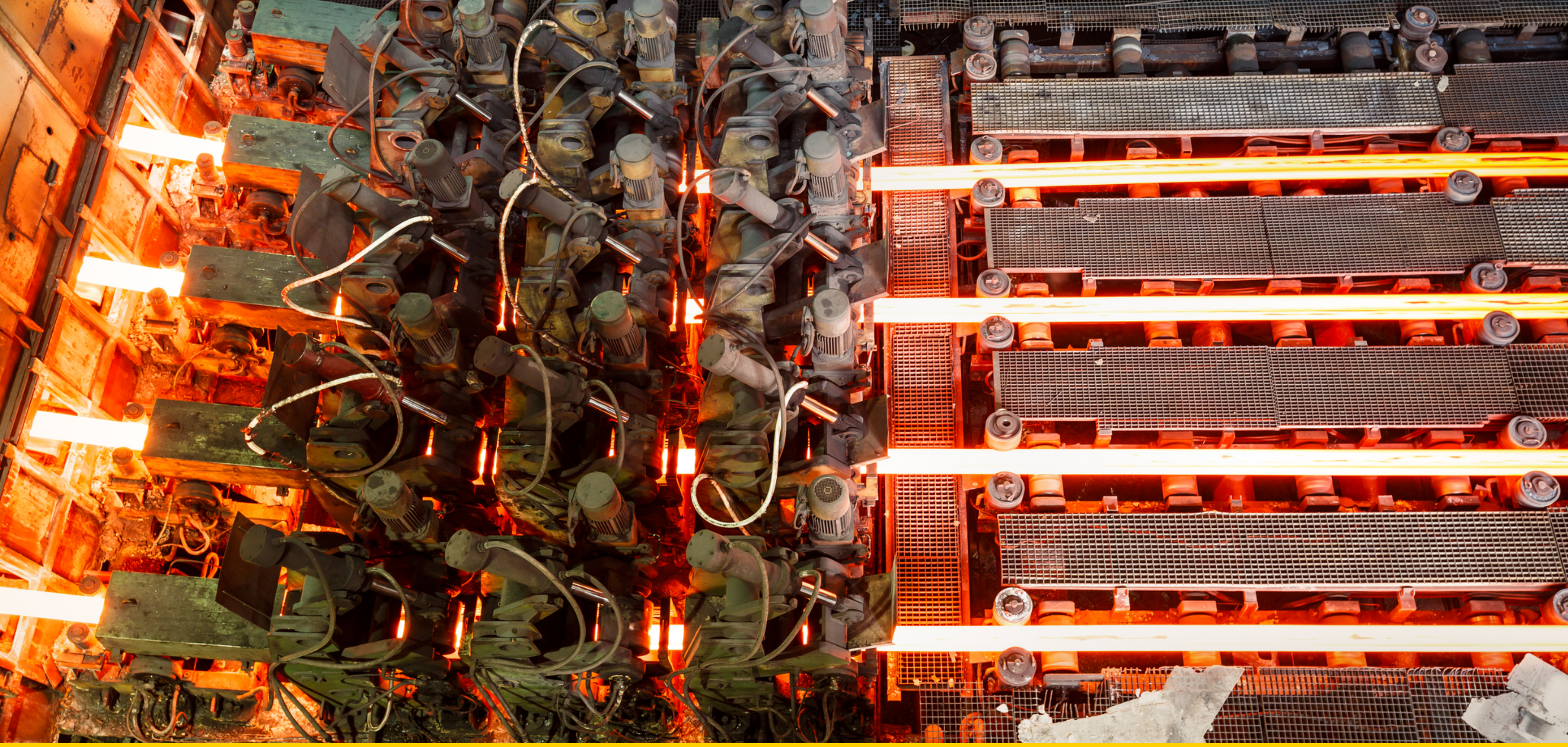
1. **Invest in critical translational research for HEA manufacturing.** A multi-agency federal research initiative is necessary to focus efforts on advancing the most promising emerging manufacturing technologies and addressing the cross-cutting barriers to commercial production and utilization. Specific attention should be paid to the following opportunities and challenges extending from design through process technologies for manufacturing at scale:

- **Alloy identification:** Better tools are needed to explore the broad design space of HEAs to identify manufacturable alloys with desired properties. Such exploration can be enabled by advancing multi-fidelity tools that link multiple layers of models and experiments, streamlining diverse tools for efficient alloy discovery, and tools that identify manufacturable refractory alloys.
- **Melting:** The complex chemistries of HEAs pose unique challenges for melting, which is a common process to combine elements to form alloys. This barrier should be addressed by extending the temperature, chemistry, and composition control capabilities of existing melt processes; developing novel electromagnetic and directed energy induction; standardizing cleaner master alloys; and enhancing analysis tools.
- **Casting:** Molten alloys are cast into final shapes or ingots for subsequent processing. Quality casting of HEAs can be realized by improving hot top casting methods, developing rheocasting methods, and advancing high-precision cooling rate control.
- **Thermo-mechanical processing and joining:** Alloys are often refined through thermal and mechanical processing to obtain desired alloy properties. Limitations of traditional processing and joining methods can be overcome by developing high-temperature roll and die materials, researching hot rolling methods that increase homogeneity of HEAs, creating “mini mills” for HEAs, and understanding the microstructural changes resulting from thermo-mechanical and joining processes.
- **Wire-, powder-, and coating-based manufacturing:** In addition to addressing challenges in melt-cast processing, R&D efforts should be focused on methods that directly form complex shapes and thin films from wires, powders, and coating methods. These methods can be realized for HEAs by advancing powder and wire production, modeling powder and coating quality, creating novel multi-material additive processes, and researching sputter coating of multiple elements.
- **Modeling:** The complexity of HEAs requires advances and benchmarking in models, including models relating microstructure and manufacturing processes to performance, models of HEA properties and processes, and models of manufacturing processes elevant to HEAs, as well as, continued development and expansion of emerging modeling methods.

2. **Establish a National Testing Center** for HEAs to develop novel high-throughput testing methods and conduct high-throughput testing for alloy discovery and characterization. Important advances would include automated massively parallel mechanical, environmental, and functional testing, such as nano-indentation, automated x-ray characterization, and parallelized shear punching. The center would work with governing bodies to develop standards and benchmarks and would house and coordinate material testing capabilities through a national testing collaboratory.

3. **Develop a central database for high entropy alloy data** that includes theoretical and experimental data on alloy properties, manufacturing processes and parameters, and models. Collected from a range of public and private stakeholders, the data will be qualified, organized, and then provided to U.S. researchers.

4. **Enhance collaborative efforts** through increased access to existing federal facilities and expertise associated with advanced manufacturing methods, characterization tools, and computing power. In addition, establish an interdisciplinary working group to provide real-time input regarding manufacturing technology roadmapping, research priorities, standards, intellectual property, technology transfer, and other issues to facilitate accelerated progress.



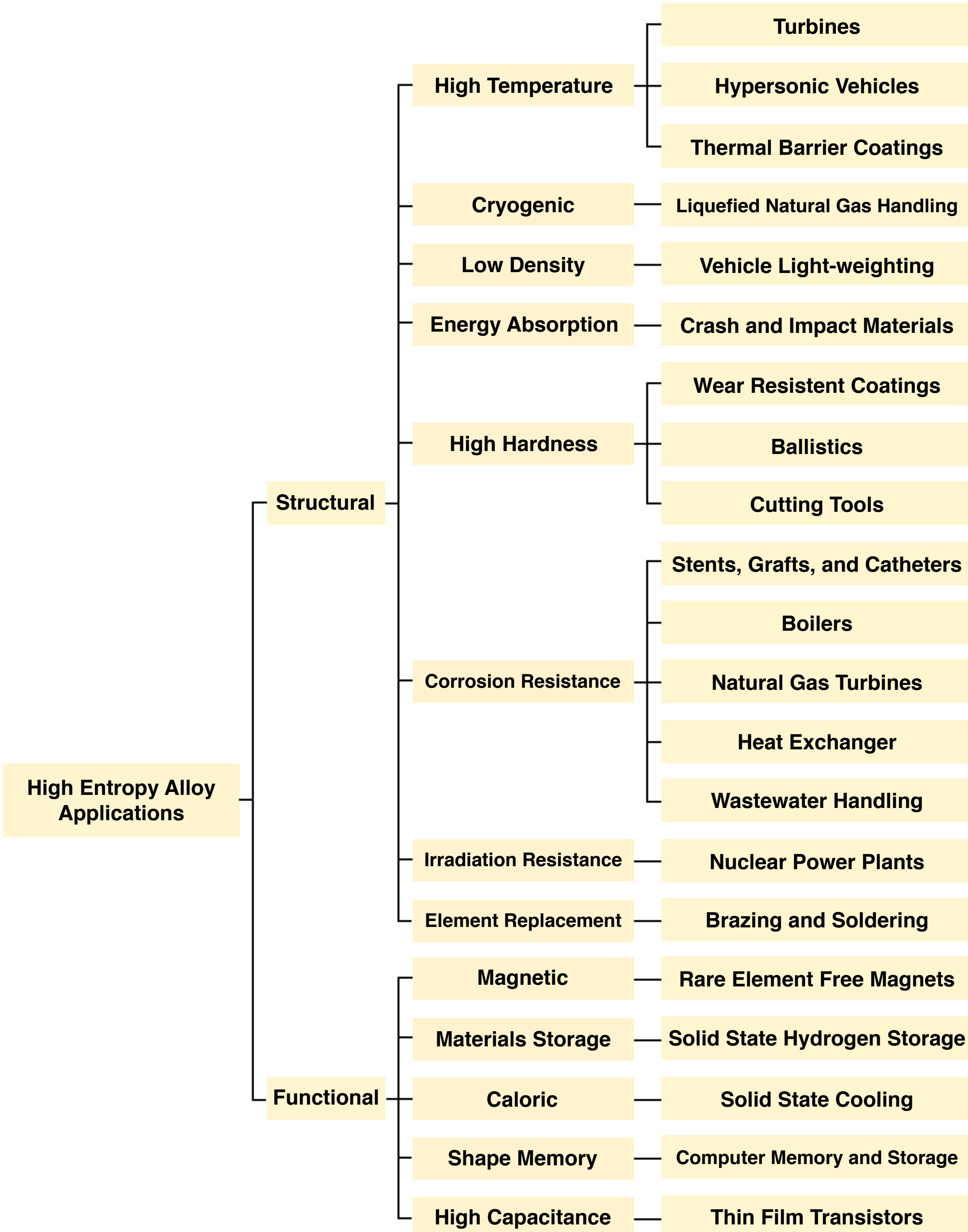
High Entropy Alloy Manufacturing Opportunities and Challenges

Around 5,000 years ago, humanity discovered that incorporating relatively small elemental additions to a base metal can dramatically improve its performance. For example, adding small amounts of tin to copper significantly improves copper's strength. Although alloying is more sophisticated today, the approach of modifying a base element with relatively minor concentrations of other elements remains largely unchanged. This approach limits available alloys to combinations that leverage only a few dozen base elements. The emerging field of high entropy alloys (HEAs), or more generally complex concentrated alloys, uses multiple base elements in roughly equal proportion. Expanding the available material set beyond compositions centered on a single base element provides a near infinite array of alloys and enables a paradigm shift from "apply the alloy you have" to "engineer the alloy you need." Researchers have created samples of HEAs that demonstrate extraordinary material performance, unique property combinations, and viability as replacements for high-cost or rare materials.[1] For this reason, HEAs are setting the stage to enable new opportunities in a cross-cutting array of applications, including those that address national priorities of security, health, and energy independence. Transitioning HEAs from laboratory-scale samples to materials and parts manufactured at scale will enable U.S. manufacturers, and our Nation, to realize this technology's value.

Cross-Cutting Potential

HEAs are expected to lead to breakthrough advances and superior performance in an array of applications across the aerospace, defense, automotive, energy, medical device, and electronics sectors, among others (Figure 1). HEAs' value often lies in the potential to offer a suite of material properties tailored to a specific application rather than superior material performance according to

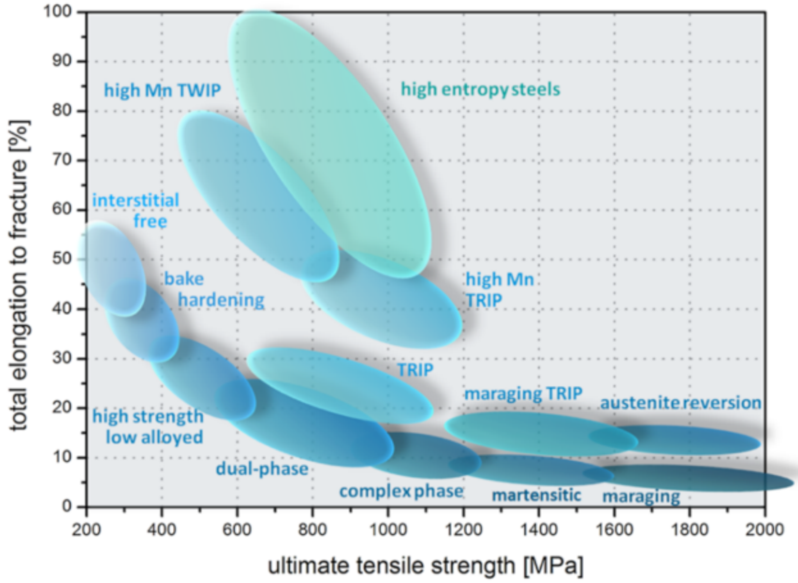
Figure 1: Advances in HEAs manufacturing technologies will impact a wide array of applications.



only a single metric. For example, high entropy steels can simultaneously provide both high elongation to fracture and high ultimate tensile strength (Figure 2),[2] a highly sought combination of properties for automotive and aerospace applications. HEAs excel in maintaining mechanical properties at both very high and very low temperatures; providing exceptional strength per weight, toughness, hardness, and corrosion resistance; and realizing challenging functional characteristics, such as magnetic, caloric, and electronic properties.

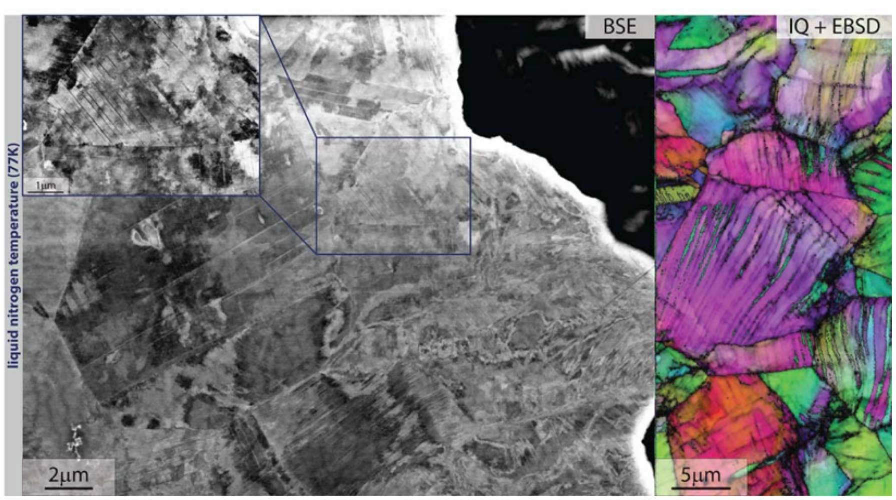
HEAs show great promise for retaining strength at high temperatures. For applications in aerospace and energy generation turbines, HEAs could generate energy savings through higher operating temperatures and increased thermodynamic efficiency.[3,4] Whereas benchmark alloys, such as Inconel 718 and Haynes 230, cannot withstand temperatures over 1100°C, HEA samples perform not only upwards of 1400°C, but also while delivering a strength of 600 MPa and specific yield strength of 50 kPa m^3 kg^{-1}.[5,6] HEAs will be critical for hypersonic vehicles that require materials that can withstand extreme operating temperatures and loads, while remaining ductile and tough. For example, samples of $AlMo_{0.5}NbTa_{0.5}TiZr$ can be strained greater than 50% before failure at elevated temperatures, which well exceed the performance of traditional alloys.[7] HEAs also show promise for next generation thermal barrier coatings for aerospace applications, potentially eliminating the need for a separate oxidation resistant coating. New HEA technologies will likely deliver simultaneous oxidation resistance and high temperature capabilities.[8]

Figure 2: High entropy steels have improved combinations of ultimate tensile strength and total elongation to fracture compared to traditional steels, which are essential properties for aerospace applications. Image courtesy of Dr. C. Cem Tasan (Massachusetts Institute of Technology).[2]



On the other temperature extreme, HEAs also present opportunities for retaining mechanical performance at cryogenic temperatures.[9,10] In applications such as liquefied natural gas handling, retention of high fracture toughness and strength at low temperatures is essential. CrCoNi alloy (a medium entropy alloy) performs comparably to the highest performance cryogenic steels at a temperature of 77K (Figures 3 and 4.)[8,9]

Figure 3: This back-scatter electron image of a medium entropy alloy at a temperature of 77K shows its strength and toughness at cryogenic temperatures. Image courtesy of Dr. Easo George (Oak Ridge National Laboratory).[8]



HEAs greatly expand the mechanical performance of metal alloys at ambient temperatures as well, including improved toughness, hardness, and density. In laboratory settings, select HEAs show exceptional impact toughness,[11,12] with potential applications in crash and impact absorption applications. High hardness materials have applications in wear-resistant coatings, ballistics, and cutting tools.[13] One HEA, AlCoCrFeNiTi, has such improved hardness over typical hard chrome plating that it can reduce wear depth by a factor of three.[14] With such exceptional mechanical performance, HEAs serve as materials for brazing and soldering, with laboratory samples demonstrating a shear strength of 220 MPa and the ability to replace harmful elements (e.g. lead) with safer alternatives.[15,16] HEAs have also introduced exciting opportunities in lightweight alloys.[17,18,19,20] Weight reduction is a priority research focus of the National Laboratories[21] and national manufacturing efforts[22] because of the potential for improved performance and energy efficiency in the automotive, aerospace, and defense sectors. For example, HEA $Al_{20}Be_{20}Fe_{10}Si_{15}Ti_{35}$ offers 3X strength per density compared to most commonly used titanium alloys in the aerospace, marine, and racing sectors (Ti-6Al-4V).[23]

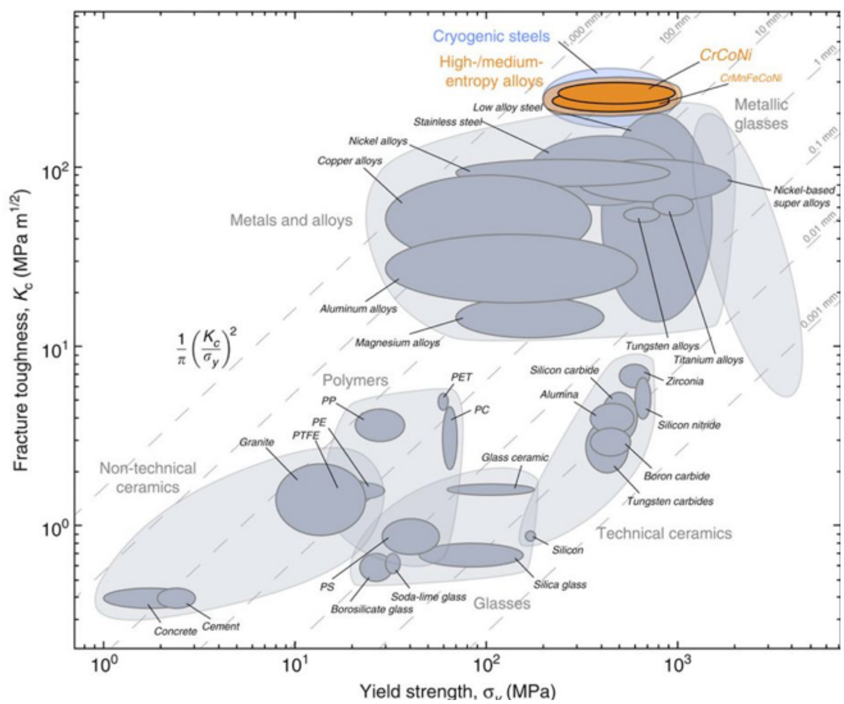


Figure 4: High and medium entropy alloys compare favorably to traditional alloys on the metrics of yield strength and fracture toughness. Image courtesy of Dr. Easo George (Oak Ridge National Laboratory).[9]

Harsh environments can deteriorate alloy performance, yet with the right combination of elements HEAs can provide exceptional corrosion and radiation resistance. These properties could be applied to a broad range of devices, for example, boilers that must withstand high temperatures, corrosive flue gasses, and slag; natural gas turbines with corrosive steam and/or CO_2; heat exchangers,which experience a host of corrosive fluids and gasses; wastewater treatment facilities; and medical devices, where corrosion resistance must be obtained in concert with fatigue durability and stiffness.[24] For example, HEA $Al_{0.1}$CrCoFeNi suffers from one-tenth the cavitation erosion of stainless steel (SS316L) in distilled water.[25] Advanced alloys are also needed for improved performance under radiation exposure. HEAs such as $Al_{0.3}$CoCrFeN have the potential to better maintain dimensional tolerance and mechanical performance under irradiation, which are essential for use in nuclear reactors.[26,27,28]

Materials are used for reasons other than their mechanical properties; early studies suggest that HEAs could also provide unique functionality in magnetics, calorics, and electronics. In the magnetic domain, HEAs could advance nuclear energy, motors, and magnetic resonance imaging through desirable combinations of magnetic saturation (for smaller, lighter components), malleability (to better form desired geometries), and resistivity (for higher efficiency performance), and the ability to be manufactured without rare or costly elements.[29,30,31,32,33] For example, HEA FeCoNi(AlSi)x ($0 \leq x \leq 0.8$ in molar ratio) has a high saturation magnetization of 1.3T (within 25% of high permeability iron alloys), a low resistivity (comparable to pure iron) of 16.7 $\mu\Omega$ cm, and a high plastic deformation of greater than

50% before fracture. Although conventional magnetic materials and metallic glasses outperform current HEAs in magnetic saturation, cost, and hysteresis, advances in HEAs may realize magnetic applications that rely on their unique combinations of properties. HEAs could advance the development of solid state cooling systems, that is, direct use of electricity to produce cooling without complicated mechanical systems through using caloric materials that change temperature on demand from electrical, magnetic, or mechanical inputs.[34,35] Federal laboratories are actively pursuing caloric materials because they enable cooling in a compact form factor with excellent reliability.[36] Researchers are also developing HEAs that can store hydrogen, providing the potential for a viable solid state hydrogen storage method.[37,38] Further, HEAs show promise for the electronics field, from thin film transistors to photovoltaics to micro-electromechanical systems (MEMS),[39] as well as shape memory[40] to realize solid state memory and storage.

The potential applications of HEAs span diverse fields and show promise to not only accelerate ecconomic growth and domestic competetive advantage, but also address pressing societal challenges. Solid state cooling, liquefied natural gas handling, nuclear degradation-resistant materials, corrosion resistant heat exchangers, and efficiency gains from high temperature performance would advance national energy goals; high-performance aerospace materials and ultra-hardness ballistics would support national security; and strong, corrosion resistant medical devices and advanced magnetic resonance imaging would help to address national health priorities.

Translating Technical Promise

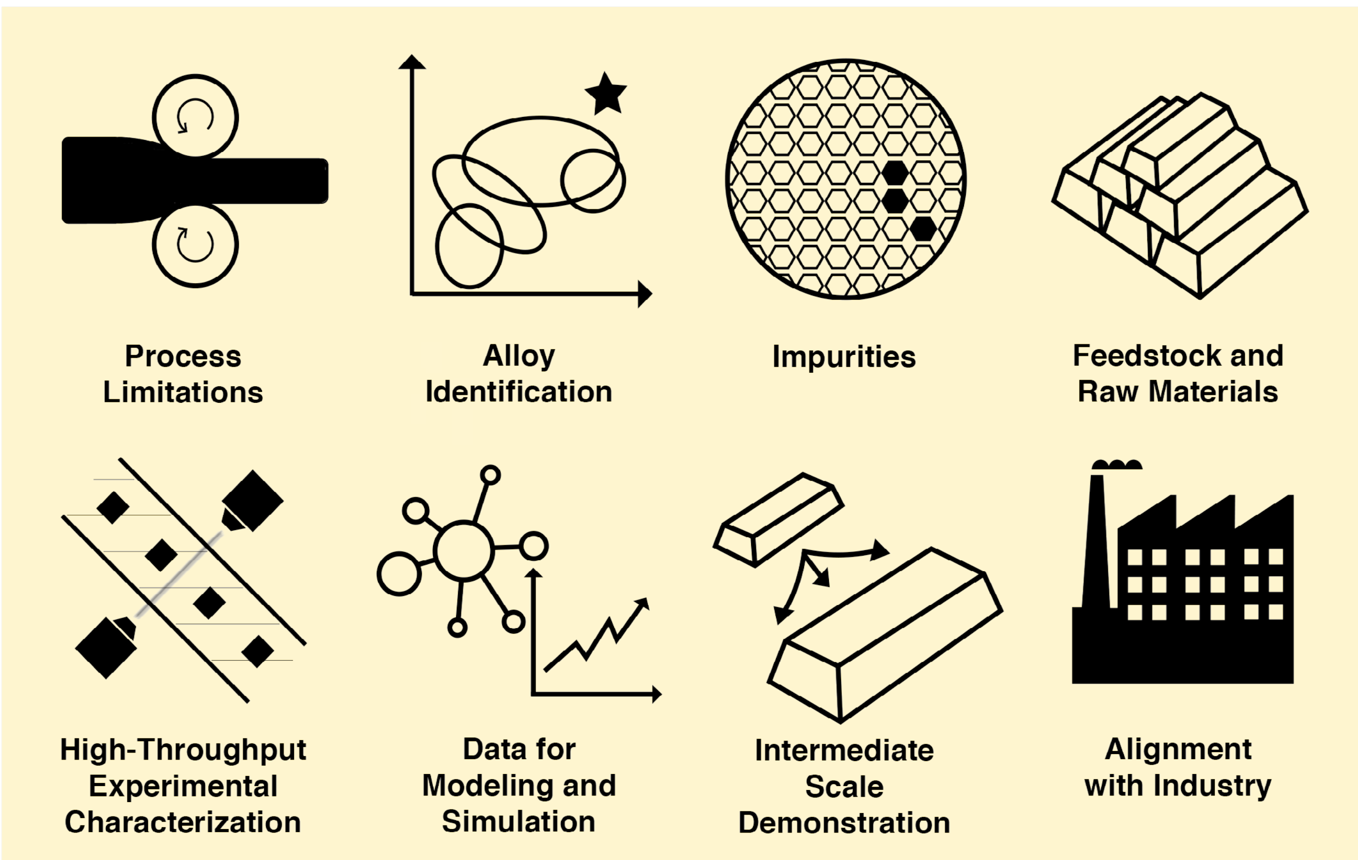
Realizing the promise of HEAs for cross-cutting impact requires translation of the emerging technologies into products manufactured at scale in the United States. The federal government has provided the critical first step by funding research on HEAs through universities, Small Business Innovation Research (SBIR) grants, and Federally Funded Research and Development Centers (FFRDCs). These efforts (detailed in the “Enhance Collaborative Efforts” section) have revealed the potential for HEAs and have created a strong base of experts, facilities, and knowledge in the United States, all critical first steps in realizing the societal and economic benefits of HEAs.

However, lab scale prototypes are not enough. A pathway is needed to bridge the good ideas and promising leads with manufactured products that leverage and bestow the benefit of HEAs. As manufacturers and HEA experts aim to bridge this gap, they are encountering cross-cutting barriers in manufacturing processes, testing, data, and access to the necessary knowledge, tools, and resources. Eight key challenges impede HEA manufacturing progress in the United States:

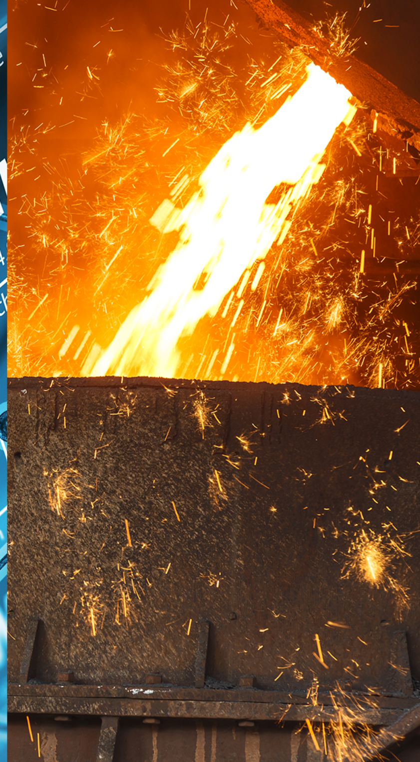
- **Process limitations:** From temperature to impurities to oxidation, HEAs pose unique manufacturing process challenges that are not yet overcome in traditional processes such as casting, thermomechanical processing, joining, and additive manufacturing.
- **Alloy identification:** To rapidly and affordably create alloys that are tailored to their needs, researchers require tools for alloy identification, modeling, and design. Current tools lack accuracy, speed, and reliability.
- **Impurities:** Current manufacturing methods cannot produce HEAs with desired levels of purity.
- **Feedstock and raw materials:** Elements, nano-particles, and master alloys are not of sufficient quality and/or too expensive for researchers and manufacturers to develop and scale HEAs.

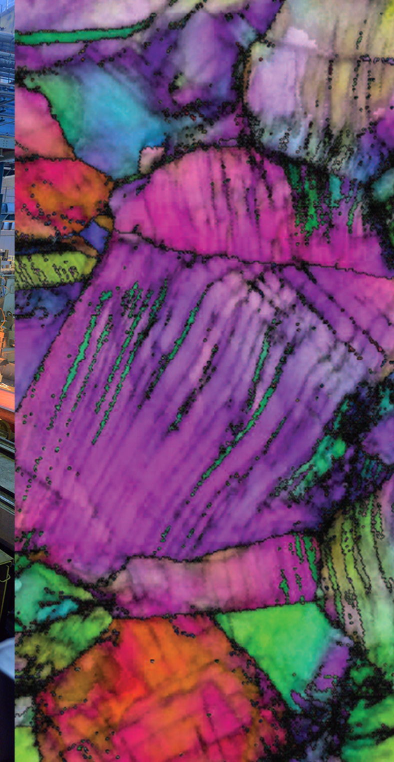
- **High-throughput experimental characterization:** Experimental characterization of alloys is critical from discovery to development to scale-up. Existing experimental equipment is either inadequate or difficult to access for researchers to characterize HEAs.
- **Data for modeling and simulation:** From understanding microstructures to optimizing manufacturing processes, data is essential to modeling and simulating HEAs, but are not yet centralized, consistent, or readily available.
- **Intermediate scale demonstration:** Although the HEA manufacturing community has made advances in producing small samples of alloys, the equipment needed to scale manufacturing processes are severely lacking.
- **Alignment with industry:** A lack of collaboration across the HEA manufacturing community creates a barrier to aligning HEA manufacturing research with the needs of industry. Resources, tools, and data are not properly shared and utilized across the community.

Key Challenges Impeding High Entropy Alloys Manufacturing Progess



To ensure that America's scientific discoveries in HEAs result in new economic opportunity and technical superiority, strategic investments and coordination are needed. MForesight: Alliance for Manufacturing Foresight convened and gathered the insights of HEA manufacturing experts from industry, academia, government, and federal labs for a workshop to begin this effort. Led by a steering committee of thought-leaders in the field, HEA experts defined and prioritized the cross-cutting challenges and explored opportunities for coordinated action by public and private stakeholders. The remainder of this report examines the challenges and opportunities facing HEA manufacturing and makes four actionable recommendations for enhancing U.S. manufacturing competitiveness in HEAs. A complete list of contributors and the workshop agenda can be found in Appendices 1 and 2.



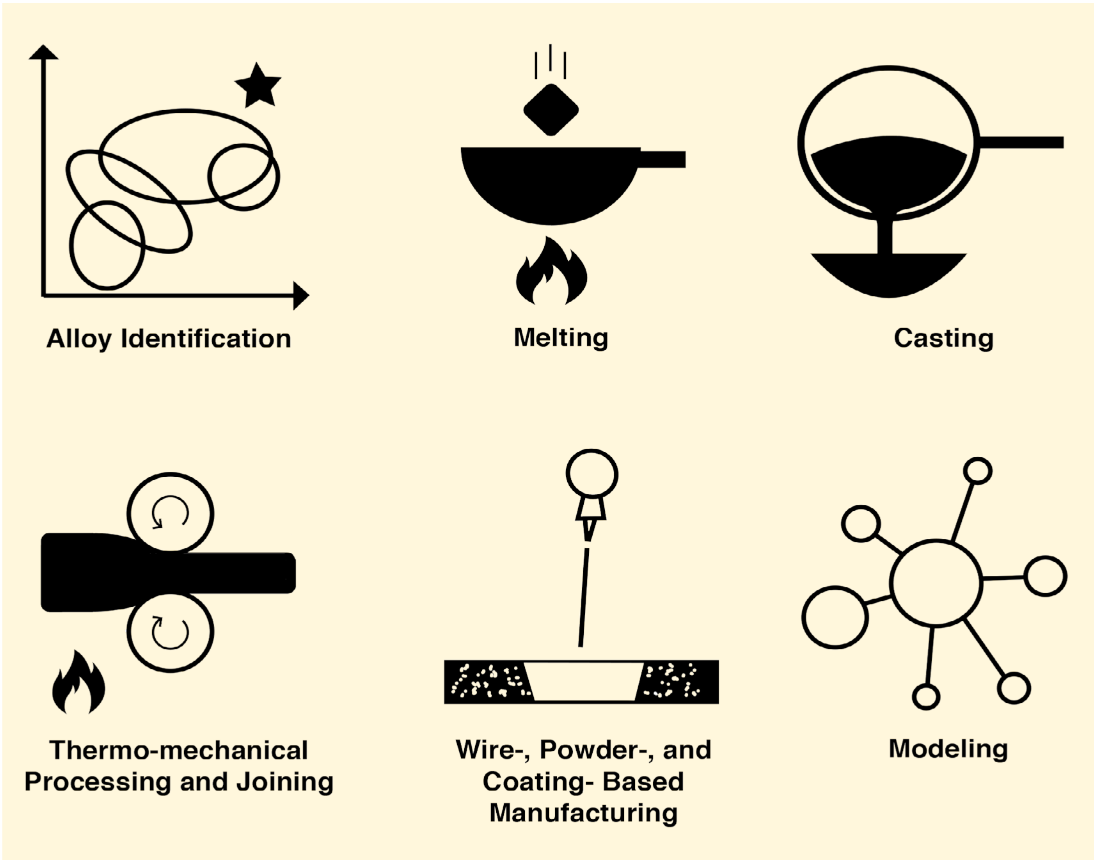


Invest in Critical Translational Research for High Entropy Alloy Manufacturing

The manufacturing of end-use products from HEAs involves a series of steps, each with a unique set of opportunities and challenges that require focused translational research. Similar to that for typical alloys, the manufacturing process for HEAs begins with the nontrivial task of identifying appropriate alloys for the specific application based on a suite of performance and manufacturability considerations. Once the alloys are identified, the next step is typically a melting process to combine the array of elements into an alloy. The alloy is then cast, sometimes into simple ingots for subsequent processing and other times into a shape resembling the final part. These cast parts are often subjected to thermo-mechanical processing (e.g., rolling, stamping, heat-treating) to modify their shape and internal grain structure. The parts can then be joined through welding, brazing, or similar processes. Complementary to traditional metals manufacturing techniques, direct shaping processes, including wire- or powder-based manufacturing (e.g., sintering, additive manufacturing) and coating processes expand the range of available geometries. Each of these processes benefits from modeling and simulation tools used to identify and optimize manufacturing parameters and alloy performance.

HEAs push the boundaries of materials science, and in the process present a wide range of unique manufacturing challenges. These include difficulties in melting together elements with vastly different properties, obtaining a desired internal microstructure during casting, and thermo-mechanical processing at new temperature extremes. Widespread use of HEAs across diverse applications requires coordinated translational research and development efforts to analyze, optimize, and verify each of the following steps in the manufacturing process.

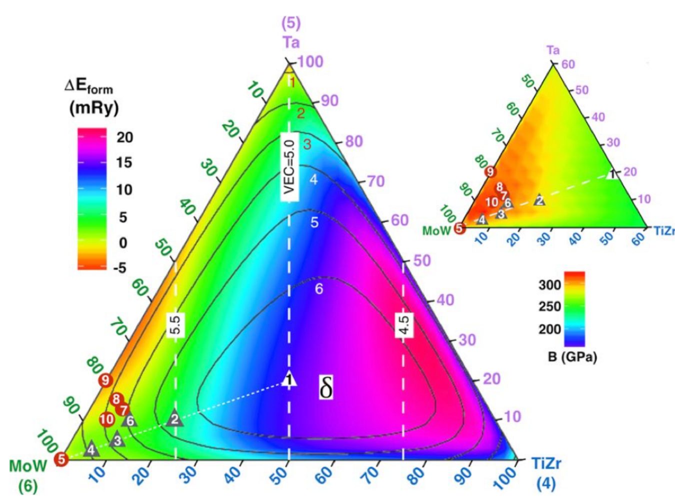
Critical Areas for Translational Research



Alloy Identification

Identifying an HEA that not only displays the optimal material properties for the application, but also can be realistically manufactured is an enormous task. The 72 metallic elements[a] can be combined in a set of 3 to 6 elements in more than 171 million ways. With a continuum of possible elemental concentrations, the options are infinite. In addition, the final microstructure of an alloy (and its corresponding properties) can rely heavily on the specific manufacturing process and parameters. Identification of useful and feasible alloy combinations is a multi-objective optimization problem. Current tools cannot span the complex design space of elemental components and manufacturing considerations. An example tool for designing concentrations of elements in an alloy for a given set of five elements is shown in Figure 5.[41]

Figure 5: A portion of a 5-dimensional design space in a design tool is used to determine the effect of changing element concentrations of an HEA. Image courtesy of Dr. Duane Johnson (Ames Laboratory).[41]



a Approximately 72 elements are considered viable candidates for alloying in that they are not radioactive, unstable, or otherwise unsuitable for inclusion in an alloy.

Realizing the potential of HEAs in the manufacturing sector relies on alloy identification tools that better balance the need for search accuracy, breadth, and speed.

The Materials Genome Initiative (MGI), a multi-agency resource and infrastructure initiative launched in 2011, aims to "discover, manufacture, and deploy advanced materials twice as fast, at a fraction of the cost." [42] Although the resources and research developed as part of the MGI have supported advancing the HEA field, ample opportunities exisit to better align MGI efforts to address the unique needs of the HEA manufacturing community, especially in the area of alloy identification. These opportunities include the following research topics:

- **Tools that link multi-fidelity layers of models and experiments** with a range of sophistication and accuracy. Computationally simple models enable rapid, low-cost alloy exploration, but are limited in accuracy and result certainty. Alternatively, rigorous experimental testing of material samples can provide high accuracy and certainty, but is slow, costly, and limited in compositional scope. Computationally intensive models paired with fast, low-cost experiments provide moderate accuracy and certainty at a moderate expense of time and costs. Research is needed to optimally connect and integrate data across these multi-fidelity layers.
- **Streamlined diverse tools for efficient alloy discovery** that connect and integrate modeling tools and data sets that are often siloed, thereby addressing only a subset of alloy and manufacturing considerations. Research should aim to enable seamless, rapid, and efficient criteria-based exploration of the composition and microstructure space while incorporating manufacturing considerations.
- **Tools for identifying manufacturable refractory alloys** that address their unique performance and manufacturing considerations. Refractory alloys made from refractory elements (e.g., tungsten, molybdenum) can withstand very high temperature and wear, but are consequently difficult to manufacture because of high or incompatible melting temperatures and difficulty in thermo-mechanical processing, among other issues.

Melting

The primary method for combining elements to form alloys, including HEAs, is melting, which involves known metallurgical challenges from contamination to oxidation to composition control. Melting for HEA production presents additional challenges, including (1) mixing elements with vastly different properties, (2) controlling unwanted phases and defects, and (3) extreme manufacturing conditions of melting (e.g., oxidation and temperature).

The wide range of elements used in HEAs often presents situations where elements will have vastly different melting and boiling temperatures, densities, and/or volatility. These differences present challenges related to composition control (elements may boil off), oxidation due to melting in air, element segregation (especially at large volumes), and defect introduction. These challenges are especially prevalent at the high temperatures required for refractory element melting and in processing HEAs used for light-weighting, where elements such as aluminum,[43] magnesium, and zinc have much lower melting and boiling temperatures than other alloying elements.[17,19,44]

Although challenged by a complex mix of elements, uniform mixing is essential to avoid unwanted defects. When HEAs use multiple master alloys (semi-finished alloys used to create the final alloy), additional defects may be introduced because the master alloys themselves may have impurities.

Although avoiding impurities is not often feasible, research is needed to understand the tolerance of HEAs to impure feedstocks.

The extreme manufacturing conditions of melting poses additional processing challenges. Preventing oxidation of elements in HEAs during mixing often necessitates use of an inert and/or vacuum melting system. However, these systems exacerbate the potential for elements to boil off, thereby preventing the easy use of traditional methods of vacuum induction melting (VIM) and/or plasma arc melting. In addition, refractory HEAs require a very high temperature to melt, and, in many cases, no suitable melt method exists for this important alloy class.

Key research areas to address these melting challenges related to HEAs include the following:

- **Extending the capabilities of existing melt processes**, including technologies for alloys with melt points higher than 1500°C, handling interstitials and complex chemistries, and advancing electromagnetic stirring for uniformity.
- **Novel electromagnetic and directed energy induction** to ensure that the molten alloy has uniform chemical composition and control of unwanted phases.
- **Standardized, cleaner master alloys** to simplify melting processes and reduce impurities.
- **Analysis tools** to relate melt processing parameters to impurity accumulation and inclusion formation.

Casting

Casting HEA melts, whether into simple ingots for later processing or into a shape resembling the final part, presents several challenges, including those typical to metal casting such as difficulty filling molds, large thermal stresses, and process repeatability. HEA properties' residence at the extremes of metallurgy creates additional hurdles. The compositional complexity of multiple elements in near-equal quantities leads to complex phase formation and solidification-path dependencies. If not appropriately managed, this complexity can result in poor-performing parts due to undesirable phase separations, the formation of brittle intermetallics, interstitial elements, porosity issues, and post-solidification phase changes. Successful casting of HEAs often requires complex solidification pathways with carefully controlled kinetics. HEA melts can also require processing temperatures that are much higher than traditional casting processes are optimized to handle.

Many of these challenges are further compounded at larger length scales. As casting processes are scaled from thin films to bulk production, obtaining uniform HEA structures, properties, and performance over large length scales becomes difficult and costly. Homogenization is especially challenging for HEAs that solidify over a large temperature range, contain refractory elements, and/or have a relatively low incipient melt temperature. Specific research areas that will enable reliable, high-volume, and high-quality casting processes for HEAs include the following:

- **"Hot top" casting[b] methods** should be expanded to address the unique solidification pathways and kinetics of HEA casting. Hot top methods include directional solidification, cold cathode electron beam melting, pressure electro slag remelting, and direct chill casting.

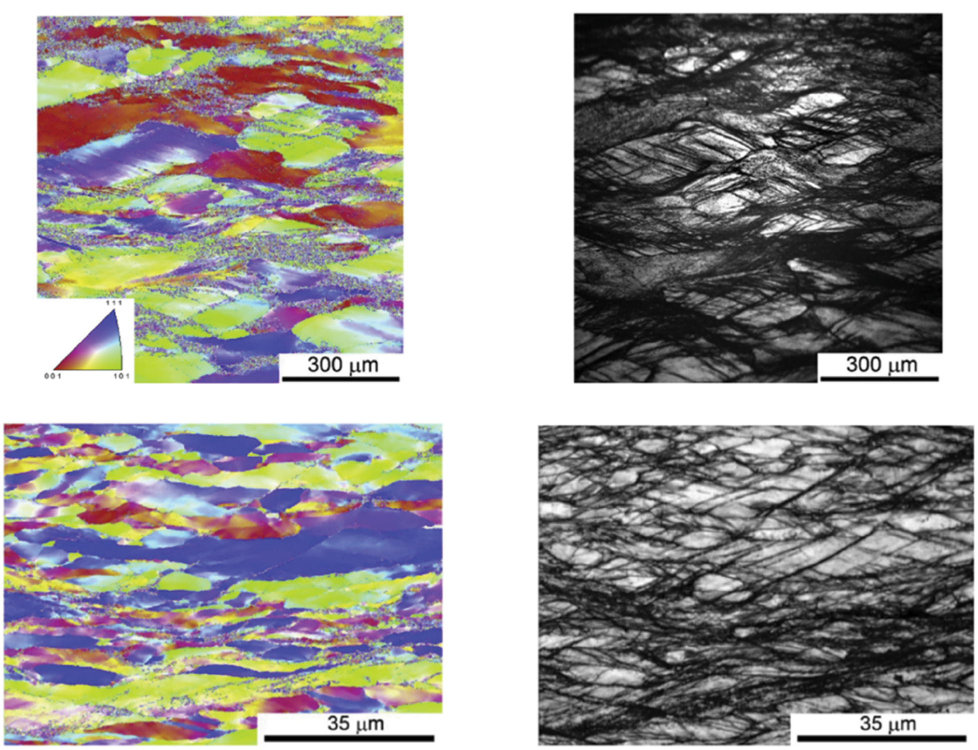
b Hot top casting involves maintaining a high temperature at the high point of a vertical casting system to ensure a constant molten metal supply at the top region of the casting. This helps prevent porosity and cracking related to shrinkage.

- **Rheocasting,** the use of semi-solid alloys in casting, should be advanced to realize the low porosity, low shrinkage, and good mechanical performance of cast HEAs.
- **High-precision cooling rate control** methods are needed across large temperature ranges to tightly control the solidification pathways during HEA casting and heat treatment to reduce porosity, segregation, and other casting challenges.

Thermo-Mechanical Processing and Joining

Thermal processing (e.g., tempering, quenching), mechanical processing (e.g., stamping, rolling), and joining operations (e.g., welding, brazing) are essential steps in creating the shape and microstructure of metal parts. Figure 6,[45] for example, shows the change in microstructure of an HEA that has undergone mechanical processing. HEAs' mixture of elements often presents challenges and operational requirements that curent manufacturing equipment cannot address. Many HEAs possess very high strength and/or are brittle, making deformation processes difficult. Several HEAs also require high-temperature (>1500°C) processing that current metal processing equipment cannot handle well. Of specific importance for high-volume mechanical processing, standard rolling mills cannot provide the extreme parting temperatures needed for high-strength HEAs. During processing such as forging or rolling, special considerations may need to be addressed to protect and control the temperature of HEAs that are oxidation sensitive or volatile. Some HEA classes have extreme work-hardening or high brittle-to-ductile transition temperatures, both of which make shaping HEAs without fracture difficult. Finally, heating involved with welding or other thermal or joining processes can destroy sensitive microstructures, which is further complicated by volatility and oxidation for low-density HEAs.

Figure 6: Electron backscatter diffraction of HfNbTaTiZr (an HEA) sheet following 65% thickness reduction (top) and 86.4% thickness reduction (bottom) show the effect of thermomechanical processing on the grain structure (Right is an image-quality map, and left is an inverse-pole-figure map for the transverse direction). Image courtesy of Dr. Oleg Senkov (Air Force Research Laboratory).[45]



Several large knowledge gaps in thermo-mechanical processing and joining prevent transition to scalable manufacturing:

- Understanding of the effect of impurities on HEA deformation is incomplete.
- Weldability and bulk properties have not been sufficiently studied to inform joining technologies.
- Process models for welding and joining HEAs are lacking.
- Overall, thermo-mechanical processing strategies for HEAs are lacking.

Additional research is needed in four key areas:

- **High-temperature roll and die materials,** including lubricants that allow for processing of high-temperature HEAs.
- **Hot rolling methods** that will increase homogeneity of HEAs.
- **"Mini mills" for HEAs,** small scale mills that produce small batches and can be started and stopped quickly to enable rapid production for testing.
- **Microstructure changes from thermo-mechanical and joining processes,** including the effect of welding, rolling, and forming.

Lightweight Innovations For Tomorrow (LIFT), a Manufacturing USA institute, focuses on advancing lightweight metal manufacturing processes and houses many important pieces of equipment for translational metal processing research. LIFT's resources and expertise could be extended to include HEA research, with lightweight HEAs as a focal point.

Powder-, Wire-, and Coating-Based Manufacturing

Not all desired HEA end products can be manufactured using melting and casting. Other techniques such as additive manufacturing, sintering, and spray coating can produce otherwise difficult or impossible geometries or compositions. These powder-, wire-, and coating-based processes present opportunities for direct additive manufacturing, greatly expanding the range of products that can be made with HEAs. Additive techniques, such as selective laser melting, can be used to produce as-built samples with high strength and ductility.[46] These methods also offer a pathway to produce complex HEA alloys in the short-term by expanding established powder production and sintering technologies.

Scaling production of powders while maintaining quality is challenging, especially for powders with multiple elements. The speed, cost, and yield, as well as the precision and control of alloy composition, surface quality, size distribution, and purity, are several hurdles that must be overcome to manufacture at scale. Refractory element powders (e.g., molybdenum and tungsten) are especially difficult to produce, because they cannot currently be produced using the hydride-dehydride (HdH)[c] process that is the standard method for other commonly used refractory elements, such as niobium, vanadium, titanium, zirconium, hafnium, and tantalum.

Combining the elements in HEAs requires the fusing of powders or and wires. Challenges to these processes include insufficient particle fusion, poorly controlled interfaces, and residual porosity. Cold spray processes, in which particles are fused together through high-velocity jetting, must address the strength, and often hardness, of HEAs, which complicates deformation for particle adhesion. With

c Hydrides are binary compounds of hydrogen with metal that create a brittle compound that can be crushed into powders of desired size.

sputter coating, an established thin film manufacturing process, coatings may vary due to varying element sputter rates and poor element mixing. Mechanical alloying provides another route to creating nanocrystalline HEAs, but existing methods may introduce impurities or disrupt microstructure when consolidating particles.[47] As a result of these factors, many alloys prove infeasible for additive processes, similar to how many alloys cannot be used in traditional metal additive manufacturing processes.

Further research is needed to realize powder-, wire-, and coating-based manufacturing methods for HEAs, including the following:

- **Advancement of powder and wire production,** which includes novel non-atomization powder manufacturing pathways, surface passivation methods, and atomization processes that excel at powder production relevant to HEAs. A focus on refractory and reactive particles is essential for HEAs and lacking in current research.
- **Model powder and coating quality,** including the relationship between manufacturing processes and alloy performance. Research should also determine the set of alloys that are viable for additive manufacturing processes.
- **Novel and emerging additive processes,** including multi-head (multi-element) and material agnostic modifications to traditional powder additive processes, as well as advances in thermal, cold spray, plasma coating, and mechanical alloying processes for HEAs.
- **Sputter coating multiple elements,** with improved control over deposition rate and mixing.[48]

Several federal research programs are addressing powder production, as well as additive manufacturing, including the America Makes Manufacturing USA center and the National Science Foundation (NSF) nanofabrication division (because many of the powders are on the nano-scale). Another key resource is the “Powder Synthesis and Alloy Design for Additive Manufacturing” project at Ames National Laboratory, which aims to improve the cost, quality, and performance of powders for additive manufacturing.

Modeling

Modeling is essential to manufacturing. Predicting and controlling process outputs enables product optimization, rapid deployment of innovations, and repeatable results. The complexity of HEAs presents both unique opportunities and unique challenges to modeling. Yet, modeling the processes, properties, and performance of HEAs is critical for their widespread application and adoption. It not only enables the identification of optimal alloys for performance and manufacturability, but also aids manufacturers in developing and scaling high-yield manufacturing processes that minimize material defects. Reliable models for HEAs are especially lacking for melting and forming processes. Insufficient understanding of solidification ranges can lead to material defects from residual stress, coring, and/or non-equilibrium phases. Modeling is needed to predict deleterious phase formation, solute entrapment, and solidification pathways, while considering various process parameters such as vapor pressure, viscosity, temperature, and length scale. For HEAs, these models must cover a broad range of elements, concentrations, and microstructures, as well as time scales appropriate the manufacturing processes. Advanced models are also needed to understand and predict the links among microstructure, performance, and failure mechanisms.

Modeling plays a key role in alloy identification, becasue computational alloy design methods often rely on advanced modeling techniques. Further, modeling aids in providing viable starting points for research efforts in HEAs. Existing and newly developed models should deliver on key metrics of accuracy, reliability, and computational speed. Key research areas that underlie HEA manufacturing include the following:

- **Manufacturing process models** relevant to HEAs, including of viscosity and diffusivity at high temperatures, the effect of welding and brazing on microstructure, energy usage, cost, and scaling laws. Reliable process recipes, standard manufacturing practices, and feasibility “scores” would also greatly accelerate the transition from models to manufactured products.
- **Models of key HEA properties and processes,** including phase and overall microstructure stability, high temperature thermodynamics, solidification pathways, oxide formation, and Hall-Petch strengthening.[d] Existing models for other alloys should be expanded to consider the structures and manufacturing processes of HEAs.
- **Models relating manufacturing, microstructure, and performance,** including the relationships between kinetics and microstructure,[49] and how the resulting microstructure alters the mechanical properties, such as ductility, fracture, toughness, and creep. Models are also needed for the relationship between interstitials and microstructural evolution (e.g,. lattice and phase stability[50,51,52]) and the resulting effect on the mechanical properties. From a manufacturing economics perspective, models are needed to evaluate the extent of impact that varying feedstock impurity levels have on alloy performance and cost.
- **Development and expansion of emerging modeling methods,** including improving the application of CALPHAD (CALculation of PHAse Diagrams) methods and tools[53,54,55] to HEAs[56,57] and improving accuracy, evaluation uncertainty, and database responsiveness. Other important emerging modeling methods include density functional theory,[58,59,60] Special Quasi-random Structure (SQS) approaches,[61] atomistic potential methods,[62] vacancy diffusivity,[63,64] ab initio molecular dynamics (AIMD),[65,66] hybrid Monte Carlo / molecular dynamics (MC/MD),[67] and Korringa-Kohn-Rostoker - Coherent Potential Approximation (KKR-CPA).[68] Other nascent methods include most-likely sub-lattice assignment, predictive approaches for free energy, and excess entropy contributions that could bring value to the field. Machine learning and deep learning present another emerging path with tremendous potential for both modeling HEA behavior and integrating with various modeling methods**.**
- **Benchmarking models** for verification and validation of their accuracy and scope. The National Institute of Standards and Technology (NIST), National Laboratories, and other FFRDCs should be leveraged for benchmarking.

d Hall-Petch Strengthening is a process to change average crystallite size to improve material strength.

Recommendation 1: Invest in Critical Translational Research for High Entropy Alloy Manufacturing focused on enabling HEA manufacturing across the following range of processes:

- *Alloy identification:* Better tools are needed to explore the broad design space of HEAs to identify manufacturable alloys with desired properties. Such exploration can be enabled by advancing multi-fidelity tools that link multiple layers of models and experiments, streamlining diverse tools for efficient alloy discovery, and tools that identify manufacturable refractory alloys.
- *Melting*: The complex chemistries of HEAs pose unique challenges for melting, which is a common process to combine elements to form alloys. This barrier should be addressed by extending the temperature, chemistry, and composition control capabilities of existing melt processes; developing novel electromagnetic and directed energy induction; standardizing cleaner master alloys; and enhancing analysis tools.
- *Casting*: Molten alloys are cast into final shapes or ingots for subsequent processing. Quality casting of HEAs can be realized by improving hot top casting methods, developing rheocasting methods, and advancing high-precision cooling rate control.
- *Thermo-mechanical processing and joining*: Alloys are often refined through thermal and mechanical processing to obtain desired alloy properties. Limitations of traditional processing and joining methods can be overcome by developing high-temperature roll and die materials, researching hot rolling methods that increase homogeneity of HEAs, creating "mini mills" for HEAs, and understanding the microstructural changes resulting from thermo-mechanical and joining processes.
- *Wire-, powder-, and coating-based manufacturing*: In addition to addressing challenges in melt-cast processing, R&D efforts should be focused on methods that directly form complex shapes and thin films from wires, powders, and coating methods. These methods can be realized for HEAs by advancing powder and wire production, modeling powder and coating quality, creating novel multi-material additive processes, and researching sputter coating of multiple elements.
- *Modeling*: The complexity of HEAs requires advances and benchmarking in models, including models relating microstructure and manufacturing processes to performance, models of HEA properties and processes, and models of manufacturing processes elevant to HEAs, as well as, continued development and expansion of emerging modeling methods.

Establish a National Testing Center

Experimental testing permeates all portions of the HEA manufacturing process, from initial alloy discovery to model development to manufacturing process refinement and validation to part qualification. As HEAs push the boundaries of materials science, they also push the limitations of currently available mechanical and functional testing. HEAs' unique compositional complexity makes them difficult to assess and characterize using traditional tools such as tomography and X-ray diffraction. No practical, time-efficient, and cost-effective methods for high-throughput mechanical testing currently exists.

Key properties for structural materials are very sensitive to both composition and microstructure. Service conditions of practical applications often require materials that exhibit a sizable set of properties, which in turn necessitates a multitude of material properties to be screened rapidly, efficiently, and often simultaneously. Wide-ranging challenges present barriers to realizing mechanical and functional testing:

- **Sample fabrication:** As stakeholders in HEA research and manufacturing have pursued testing options, they have encountered difficulty in fabricating high-quality samples (including both stable and meta-stable) to eliminate testing uncertainty based on sample variation.
- **Size scale:** Experimental methods cannot always provide key measurements at size scales small enough to enable high-throughput experiments, especially in the key areas of tensile strength and ductility. Mechanical properties are sensitive to length scale, which introduces another technical challenge in coupling testing methods, such as thin film, liquid, powder, and large scale, to inform comprehensive understanding of the properties.
- **Complex testing:** Mixing test requirements (e.g., complex loading, environmental interactions) has proven difficult, as has assessing properties in high temperature environments. Figure 7 shows an example of HEA testing at multiple temperatures, which is critical for testing cryogenic applications.[8]

- **High-throughput:** High-throughput computational capabilities to predict equilibrium phases and phase diagrams are advancing rapidly and are already making important contributions, but serious deficiencies still require high-throughput experiments to evaluate phase equilibria. The resultant major gap in critical data continues to block progress in modeling, simulation, and alloy identification.
- **Standardization:** Testing and the resulting data are not consistent, with a lack of common taxonomy and consistent language among diverse stakeholders. In addition, reliable standards around chemical verification for these complex alloys are lacking. Figure 8 shows how HEAs can be compared using the same testing protocols.[69]

A National Testing Center can serve as a research hub for novel testing methods, a centralized resource for U.S. researchers and manufacturers to perform high-throughput testing of their materials, a coordinator of unique materials testing capabilities, and a catalyst to develop enhanced standards, certifications, and benchmarks.

Figure 7: The impact of environmental conditions, such as temperature, is shown by the fracture surfaces. (A) Stereomicroscopic photographs of CrMnFeCoNi (an HEA) that has been fractured. (B) SEM of the fracture surface. Image courtesy of Dr. Easo George (Oak Ridge National Laboratory).[8]

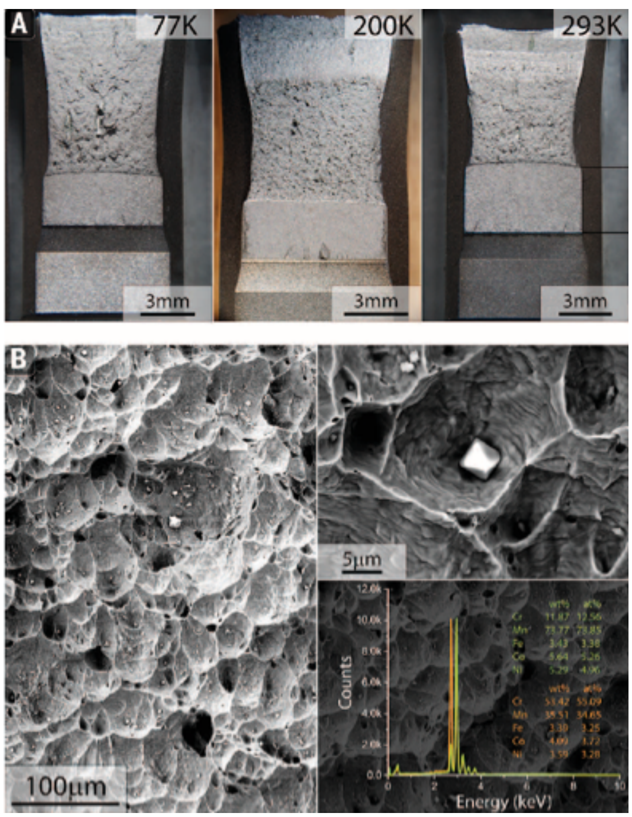
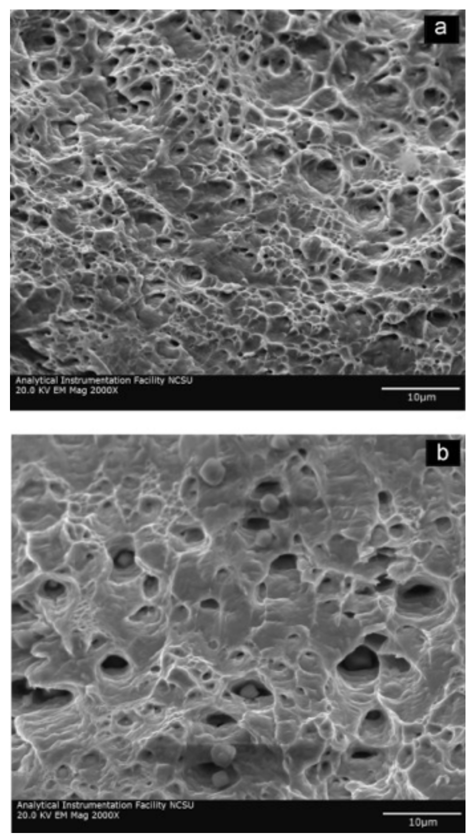


Figure 8: The impact of adding a single element is shown by the highly differentiated fracture surface. Electron images of (a) NiFeCrCo and (b) NiFeCrCoMn are shown at their fracture surfaces. Image courtesy of Dr. Carl Koch (North Carolina State University).[69]



Novel High-Throughput Testing Methods

Novel high-throughput testing methods, and the supporting sample preparation, are needed to determine a range of mechanical, material, environmental, and functional properties. To enable this testing, material preparation methods should be developed to provide the versatility, quality, and quantity necessitated by high-throughput testing. Clean, precise compositions could be enabled by the development of a powder production system to create small quantities (i.e., 10g) of desired alloys for testing. A "candy-dot" concept may be an effective route, where the materials library consists of an array of physically separated columns—each with a distinct composition that may include completely different elements from those found in adjacent columns. This "alloy-on-demand" materials library will require new processing methods; advances in additive manufacturing may help to address this challenge.

High-throughput tests for structural HEAs introduce new technical challenges for materials libraries. Current materials libraries typically use controlled composition gradients in thin films as well as much thicker diffusion multiples.[e,70] However, because materials libraries for structural materials also evaluate microstructural features, libraries with controlled microstructural gradients must be devised and implemented. Many microstructural features can have a strong influence on mechanical properties, including grain size; the size, volume fraction, and distribution of "second-phase" particles used for strengthening; phase aspect ratio and orientation; and crystallographic texture. Approaches to produce materials libraries with controlled gradients for each of these microstructural features are needed. New high-throughput tests for HEAs should be devised, designed, and reduced to practice. Sample preparation that replicates manufacturing processes, such as cold working, is also essential for testing, driving the need for research on micro-forges that can replicate cold-forming processes.

Translating traditional material testing methods to small-scale, massively parallel methods will be essential for enabling high-throughput and localized testing. Challenges associated with designing and building test equipment include the ability to locally apply and measure load, displacement, and temperature in an automated, parallelized fashion. Important equipment and tests in this area include parallelized miniature shear punching (and the associated assessment), whole plate X-ray and environmental testing that can be used on diffusion multiples, and massively parallel nano-indentation.

NIST has advanced many of these methods, especially through the MGI's "Data on Demand"[71] project and the Material Measurement Laboratory.[f] The HEA manufacturing community has identified a multitude of properties for which current testing methods are inadequate for high-throughput HEA assessment including the following:

- **Mechanical:** Simultaneous measurement of strength and ductility, simultaneous creep and fatigue, fracture toughness, creep, elastic modulus, and parallelized ductile to brittle transition temperature (DBTT) measurements.
- **Material (chemical and microstructure):** Radial distribution function (RDF) order and structure, as well as intermediate-scale homogeneity.
- **Environmental:** High-temperature performance, rapid oxidation testing, and response to irradiation.
- **Functional:** Thermal, electric, magnetic, and magnetocaloric.

High-Throughput Testing for U.S. Researchers

To meet the overall goal of scaling HEA production in the United States, the National Testing Center

e Diffusion multiples are blocks of materials with systematic grading of three or more elements, allowing the study of many different element combinations.
f https://www.nist.gov/mml

could provide a suite of advanced materials testing equipment, data, and expertise to U.S. researchers, especially small and medium-sized manufacturers.

Although some high-throughput testing is already well-established for functional materials, the equipment needed to manufacture a wide array of sample alloys and to run high-throughput evaluations is expensive, creating a barrier to entry. The equipment—especially for material testing—is often unique, requiring staff with specialized training and experience. These challenges limit the number of research institutes that can operate and maintain a high-throughput testing facility, thereby restricting more widespread use of this methodology.

Through a public-private funding model, affordable access to otherwise cost-prohibitive equipment can be made available. This equipment includes both established materials testing tools, as well as novel high-throughput tools developed at the center. Examples include Charpy impact tests, impact hammers, punch tests, and fatigue testing. To accelerate material testing, material creation tools should also be included at the Center, such as libraries of common alloys and custom material production capabilities.

Materials Testing Collaboratory

A distributed, yet highly connected collaboratory[g] is needed to unify disparate and distributed testing resources. Although many capabilities still need to be developed, this highly connected network would provide HEA researchers with access to the full range of national talent and facilities residing at universities, National Laboratories, and other FFRDCs. These resources complement the capabilities of the recommended High-Throughput Testing Center. A major advantage of this approach is that individual technical challenges can be addressed at institutes whose capabilities and interests best align with that challenge. By linking all the activities to a single collaboratory, HEA funding, researchers, and research challenges can be quickly connected to the appropriate equipment, resources, and expertise.

Having determined the need for this collaboratory for high-throughput testing,[72] NIST is in the early stages of its organization.[73] The NIST collaboratory is not exclusively focused on HEAs, but rather on addressing high-throughput testing broadly. Further, the NIST collaboratory does not address new high-throughput tests needed for structural properties. Nevertheless, the technical challenges identified in this report are fully compatible with the challenges to be addressed in the NIST collaboratory. The NIST High-Throughput Experimental Materials Collaboratory project should be developed and expanded to address the needs of the HEA community. Examples of resources[h] that would benefit the HEA community include the following:

- **Alloy sample creation:** Ames Laboratory Materials Preparation Center (MPC) and the Oak Ridge National Laboratory (ORNL) Manufacturing Demonstration Facility (MDF).
- **Characterization:** Ames Laboratory Sensitive Instrument Facility (SIF), ORNL Neutron User Facilities, Department of Energy (DOE) hard X-ray synchrotron facilities, as well as an array of tools and instruments housed at NIST.
- **Modeling and analysis:** The NIST MGI and NIST OpenCalphad,[74] which is free, open source software for calculating thermodynamics of multicomponent systems.

g A collaboratory is a virtual laboratory that connects researchers, tools, data, computational resources, and information for physically disparate locations.
h For more information on these resources and many others, see the Enhance Access to Federal Resources section of this report.

Enhance Standards, Certifications, and Benchmarks

A lack of standards and benchmarks related to testing procedures, materials quality, and acceptable values restricts the ability of HEA researchers to perform, evaluate, and synthesize testing. Advancing work in these areas is critical to HEA manufacturing from discovery to validation. The HEA community highlighted nine key areas as needing national attention:

- Correlation of high-throughput measurements of thin films with the resulting properties in bulk materials
- Correlation of low-temperature testing to high temperature testing, towards accelerating efforts and decreasing costs
- Uncertainty analysis of common testing methods as they relate to realized mass production performance
- Common taxonomy and language for testing and the resulting data in HEAs
- Standards for chemistry verification in HEAs
- Standards for non-destructive evaluation results for qualification and certification of HEAs
- Standard and accepted definitions for feedstocks (both powder and wire) to define critical parameters for measurement and specification
- Standardize measurement automation
- Established benchmarks for HEA manufacturing processes

Recommendation 2: Establish a National Testing Center for HEAs to develop novel high-throughput testing methods and conduct high-throughput testing for alloy discovery and characterization. Important advances would include automated massively parallel mechanical, environmental, and functional testing, such as nano-indentation, automated x-ray characterization, and parallelized shear punching. The center would work with governing bodies to develop standards and benchmarks and would house and coordinate material testing capabilities through a national testing collaboratory.

Develop a Central Database for High Entropy Alloy Data

Data has proven to be one of the most valuable assets for advancing both materials science and manufacturing. This holds true especially for HEA manufacturing, where data is essential for alloy discovery, manufacturing optimization, and material validation. Transitioning HEAs to scaled manufacturing requires that data be collected, compiled, analyzed, and accessed in a coordinated and optimal manner. A central database with coordinated protocols would allow the HEA manufacturing community to accelerate progress, realize improved performance, and rapidly deploy new alloys. A central database is needed for HEA manufacturing development to advance in five important ways:

- **Avoid duplicate efforts:** Avoid each individual research group conducting redundant literature reviews to understand the state of the field.
- **Expand analysis methods:** Enhance the ability to use advanced analysis such as machine learning to drive HEA design; many of these techniques rely on large quantities of data.
- **Expand complex models:** Improve mechanistic modeling capabilities; physical trends may only be apparent from comprehensive data analysis. This is especially important for chemical and thermodynamic data in phase diagrams.
- **Consider unfavorable results:** Unfavorable results are not always published, yet they are critical to advancing the field and ensuring efficient resource allocation.
- **Accelerate progress:** Data is often generated at high rates through experiments and equipment (e.g., synchrotrons), and analysis must keep pace.

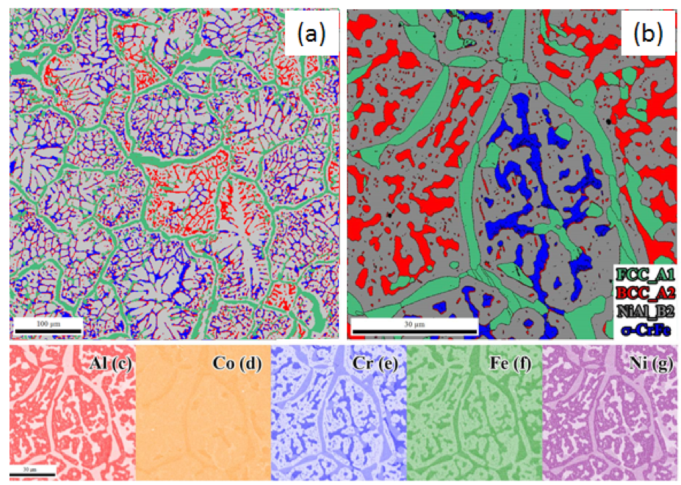
A central database to collect, organize, and share HEA test data from a multitude of sources would empower U.S. researchers to coordinate efforts and accelerate innovation.

Data Types to Collect

The central database should focus on the following types of data most relevant for scaling HEA production:

- **Alloy properties:** Composition, microstructure, elastic modulus, diffusivity, tensile strength and ductility, fault energies, thermal conductivity, thermal expansion modulus, density, irradiation resistance, oxidation resistance, shock properties, common impurities, and a range of other standard physical and functional material properties. An example of composition and microstructure is shown in Figure 9.[75]
- **Manufacturing methods and parameters:** Processing provenance, supplies, scale, hearth size, electrode size, melt stock, crucible types, melt modes, atmospheres, hot working information such as dies, lubricants, and strain rates, and machining information such as speeds and lubricants used.
- **Models and simulations:** Density functional theory databases, customized thermodynamic databases, viscosity models, Monte Carlo simulation data, and the results of thermodynamic and other simulations.

Figure 9: Electron backscatter diffraction and energy dispersive X-ray spectrometry is used to phase map AlCoCrFeNi-HP, an HEA with high strength per weight. Characterization of elemental distributions is important to understanding alloy structure and performance. Image courtesy of Dr. Peter Liaw (University of Tennessee, Knoxville).[75]



Data Collection

Beyond published literature, it will be important to mine data from unpublished efforts at universities, FFRDCs, the MGI, existing databases, and other HEA efforts mentioned in this report, such as the National Testing Center. Existing federal laboratory collaborations, such as LightMAT,[i,76] could also accelerate the data collection and curation processes.

Technical and policy measures will advance data collection. On the technical side, the incorporation of existing published literature will require a concerted effort from the HEA community to re-examine, classify, and compile data. Regarding future data, a system of automated post-processing of data could be incorporated into the centralized platform to perform automatic, standardized analysis, while ensuring that the data is entered into the database. On the policy side, requiring entities that receive federal grants to provide their data to a federal database would ensure continuity of access to data, as well as the range of benefits offered by a centralized database. Policy at the federal level to ensure that federal laboratories report their non-confidential data to a central database is vital to accelerating data collection. Other policy measures include "data for access," wherein access to the database is

i LightMAT is the National Laboratories lightweight materials consortium that connecs national laboratories, industry, and academia to computing, synthesis, and characterization tools and expertise for lightweight materials.

contingent on providing additional data. A final method is sponsored extraction, where an entity (public or private) sponsors the extraction of data from literature to the database in the technical area of its choice.

Throughout the data collection process, several considerations should be addressed to ensure that the database is of high quality and meets the needs of all stakeholders:

- **Delayed publication:** On the academic side, a time-lag should be implemented to enable researchers to publish or patent results before they become public through the database, even if the data were submitted prior to publication or patent filing.
- **Data agnostic:** Data collection must be agnostic, that is, avoiding choices that would bias the data included in the database.
- **Ensure sharing of all data:** The sharing of "bad" data that does not yield favorable results should be encouraged, because such data is essential for accelerating progress and ensuring robust data sets.
- **Identification of gaps:** Systematic overview of the data should be performed to identify critical gaps of information.
- **Information protection:** The needs of industry to protect its data should be balanced with the need to provide a comprehensive and open database.

Data Qualification

The accuracy and thoroughness of the data in the database should be ensured through qualification measures. Five methods can be used to qualify this data, although a hybrid approach will likely yield the best results:

- **Machine learning** has been shown to be a very helpful tool in data qualification and curation;[77] it can quickly identify likely outliers for expert review.
- **The involvement of experts,** including modelers and experimentalists in processing and characterization, in data collection and qualification will create a feedback loop to the data submitters, improving overall data quality.
- **The creation/development of standards for data pedigree** and provenance will encourage use of existing data and will improve the understanding of the data reliability, generalizability, and validity.
- **The pedigree of historical/archival data** passed uncorrupted into modern databases will ensure that data context and limits are not lost or misinterpreted.
- **User rating of the credibility of the data** and the pedigree enables a crowd-sourced assesment of data quality.

Data Organization

Organizing data is important for both analysis and access. Standardization of materials data has converged on the Physical Information File (PIF), which is an open-source JSON[j]-based schema for

j JSON (JavaScript Object Notation) is a common, language-independent data format for transferring information in an array format.

storing hierarchical materials data.[78] A small group of HEA domain experts could make reasonable choices regarding standardization of HEA data within the PIF. As the database is developed, alloy families must be categorized to a precision level such that properties and challenges among particular alloy families are not incorrectly translated to challenges for all HEAs. In addition, much like for medical data, anonymization methods are needed protect the sources of some data, especially those from industry. The organized data can be processed to provide benchmarks for validation of model predictions, as well as tractable data visualizations.

NIST (often through the MGI) has advanced efforts on materials data collection, organization, and analysis, including the "Materials Data Curation System,"[79,80] the "Machine Learning for High Throughput Materials Discovery and Optimization Applications" project,[81] the "Interatomic Potentials Repository" project,[82] the "Materials Data Facility,"[83] the "Materials Data Repository,"[84] and the "Materials Resource Registry."[85] These efforts should be expanded to address the array of data essential to scaling HEA manufacturing detailed in the "Data Types to Collect" section.

Data Access

Methodologies for managing access to the database could fall into one of four types: open-access, fee-for-access, data-for-access, or mixed. Modern materials data platforms, such as Citrination,[86] offer granular permissions that control data access at the individual, group, and global levels. One potential method to enhance industry access is to partition the database to provide companies with only data relevant to them. In this way, companies can lock down newly generated data to protect intellectual property while benefiting from the database. More broadly, the database would benefit greatly from a pre-competitive, open-source data policy, with the potential to add an incentive to contribute, such as requiring data contributions for database access. Finally, the materials data infrastructure community has made great strides in developing interoperable application programming interfaces (APIs)[k,87,88] which could also be adopted by software packages such as Pandat by Computherm.[89]

Recommendation 3: Develop a central database for high entropy alloy data that includes theoretical and experimental data on alloy properties, manufacturing processes and parameters, and models. Collected from a range of public and private stakeholders, the data will be qualified, organized, and then provided to U.S. researchers.

k An API is a set of tools and protocols that enables easy and clearly defined communication between software components or systems.

Enhance Collaborative Efforts

The research efforts, experts, and resources that could assist the HEA manufacturing community are siloed within a multitude of locations, projects, and agencies. Measures are needed to bridge the gaps and encourage collaboration on common challenges and opportunities.

Enhance Access to Federal Resources

Private-sector research in HEA properties and manufacturing processes often occurs at small firms with limited access to the full range of appropriate resources. Computing power for sophisticated modeling and simulation, test equipment and material characterization tools, and advanced manufacturing equipment are often too costly for small firms. Although a small firm may recognize the commercial opportunity presented by a new alloy, its ability to develop, characterize, manufacture, and test the alloy frequently will depend on its ability to partner with a research organization, such as a university or federal laboratory, with the requisite equipment and capabilities. Many of the needed resources are available at outward-facing FFRDCs, which also, fortunately, often have programs to encourage and facilitate access by industry.

Federal Facilities

Several outward-facing federal laboratories have equipment, high-performance computing, materials synthesis and characterization capabilities, and specialized expertise that can be applied to HEA development, including manufacturing processes. Collaboration amoung the experts in these laboratories and the industrial and academic researchers working on HEAs would accelerate the translation of promising HEAs to commercial production. Relevant facilities include the following:

Ames Laboratory has expertise in metal synthesis, characterization, design, and development, as well as theoretical expertise in alloy design and development, plasticity simulation, solidification, and materials informatics. Specific facilities, programs, and projects of interest include the following:

- **The Materials Preparation Center (MPC)**[l] is recognized for its unique capabilities in purification, preparation, and characterization of metals, alloys, and single crystals, especially rare earth metals and alloys. MPC provides R&D quantities of high-purity materials (up to 25 kg) and unique characterization services to scientists at university, industry, and government facilities on a cost-recovery basis. Technologies include (1) metal synthesis (rapid solidification by free-jet melt spinning, crucible melt/bottom pour/chill casting, melt levitation/splat quenching, and arc melting/chill casting), (2) powder atomization (high-pressure gas and rotating disk) technologies for aluminum, magnesium, nickel, iron, cobalt, and rare-earth alloy powders, (3) rapid assessment methodologies using high-throughput bulk combinatorial synthesis of large libraries of materials to discover new materials by additive manufacturing directed-energy deposition technology using multiple metal powders, and (4) an in-house developed combinatorial arc melting system capable of producing 128 bulk samples per day.
- **The Sensitive Instrument Facility (SIF)**[m] features current state-of-the-art and next-generation electron-beam characterization capabilities to study materials structure and chemistry (surface and bulk) at the atomic scale, housed in a thermal-, vibration- and electromagnetic-free environment, and sample preparation laboratories, taking characterization from start to finish.
- **The CaloriCool**[n] consortium designs, discovers, and deploys high-performance, reversible, caloric energy-conversion materials that can be adopted economically by industry for a new generation of energy-efficient solid-state cooling or heat-pumping devices and systems. HEAs have demonstrated functional properties that show promise in this area.[90]
- **The Critical Materials Institute (CMI)**[o] focuses on technologies that make better use of materials (especially rare earth-based) and eliminate the need for materials that are subject to supply disruptions but are essential for U.S. competitiveness in clean energy. CMI features research, applications, and deployment to U.S. industry for ways to diversify supplies of critical materials, develop substitutes, improve reuse and recycling, enable research, sustain the environment, study the supply chain, and analyze economics.
- **The Mapping and Manipulating Phase Transformations Pathways** project focuses on designing alloys and controlling phase transformation from electronic structure-based thermodynamic methods.
- **The SMARTER Project** (Science of Multicomponent Alloys—Roadmap for Theoretical and Experimental Research) for high-temperature HEAs focuses on comparing experiment and theory and improving oxidation resistance.
- **The DREAM Project** (Development of Radically Enhanced alnico Magnets (DREaM) for Traction Drive Motors) works to design and synthesize high-energy product permanent magnets in bulk final shape without using rare-earth elements.
- **The Powder Synthesis and Alloy Design for Additive Manufacturing** project focuses on improving additive manufacturing feedstock powder synthesis and alloy design by advancing gas atomization technology and designing metallic alloys that can develop optimum properties from processing by electron beam and laser-based AM methods.

l https://www.ameslab.gov/mpc
m https://sif.ameslab.gov
n caloricool.org
o https://cmi.ameslab.gov

The Oak Ridge National Laboratory (ORNL) User Facilities provide access to advanced experimental and modeling tools, typically cost-free if the research is intended for publication in the open literature. Examples from ORNL that align with HEA research include the following:

- **The Industrial Applications Program**[p] promotes industry engagement with two of the most powerful neutron science facilities in the world—the High Flux Isotope Reactor and the Spallation Neutron Source.
- **The Neutron User Facilities**[q] includes (1) engineering diffractometers equipped for in situ studies of mechanical and phase transformation behaviors, (2) non-destructive 3D imaging (computed tomography) of large, bulk parts to detect defects, cracks, porosity, and composition inhomogeneity (3) in-situ diffraction and imaging studies of casting, welding, and operational devices (combustion engines, heat exchangers, fuel injectors, batteries) and (4) tools for local and long-range crystal order, magnetic order, and vibrational spectroscopy.
- **The Center for Nanophase Materials Sciences**[r] integrates nanoscale science with neutron science, synthesis science, theory, modeling, and simulation. The center provides access to electron and atom-probe microscopy, scanning probe microscopy, and nanofabrication facilities.
- **The Manufacturing Demonstration Facility (MDF)**[s] provides access to R&D expertise, facilities, and tools to facilitate rapid adoption of advanced manufacturing technologies, potentially those involving HEAs.

NIST has multiple programs that underlie HEA advancements:

- **Open Calphad**[t] develops software tools for the CALPHAD method, which has proven to be a key modeling method for HEAs.
- **The Materials Design Toolkit**[u] provides a framework for integrating a variety of software tools, including OpenCalphad and optimization tools towards Integrated Computational Materials Engineering (ICME).
- **Additive Manufacturing**[v] offers a wide array of research in additive manufacturing processes and models that could be leveraged for HEA manufacturing.
- **The Cobalt Based Superalloys project**[w] has developed HEA relevant process modeling and microstructure prediction tools.

The National Energy Technology Laboratory has an array of capabilities and facilities for development and testing of HEAs.[x] Efforts are focused especially on development and manufacture of materials for extreme environments (e.g., combinations of mechanical stress with corrosive and erosive environments).

- **The Severe Environment Corrosion and Erosion Research Facility** and related laboratories assess materials performance in simulated service conditions at high temperatures and high pressures.
- **The Mechanical Testing Laboratory** has fatigue and creep testing capabilities.

p http://swc.ornl.gov/industry
q https://neutrons.ornl.gov/
r https://www.ornl.gov/facility/cnms
s https://www.ornl.gov/mdf
t https://mgi.nist.gov/opencalphad
u https://mgi.nist.gov/materials-design-toolkit
v https://www.nist.gov/topics/additive-manufacturing
w https://www.nist.gov/programs-projects/data-and-computational-tools-advanced-materials-design-structural-materials
x https://www.netl.doe.gov/research/on-site-research/research-capabilities/research-facilities

- **The Alloy Fabrication Laboratory** contains facilities for melting, casting, forging, rolling, and heat-treating materials from a few grams to 100 kilograms.

The Argonne National Laboratory Advanced Photon Source[y] is a synchrotron source for X-ray beams, which are important for materials research and characterization.

The Department of Energy (DOE) Energy Materials Network[z] provides a consortium of resources and expertise focused on advanced functional materials. Many of the focus areas can be addressed with HEAs, such as next generation electrocatalysts.[91]

The Manufacturing USA institutes, including LIFT,[aa] Digital Manufacturing and Design Innovation Institute (DMDII), and Clean Energy Smart Manufacturing Innovation Institute (CESMII), have translational research resources that can be leveraged in scaling of HEA manufacturing. LIFT has resources in materials processing, including shaping, joining, and materials light-weighting. DMDII has technologies for spanning the junction between physical manufacturing, design, and data. CESMII has resources for extracting and analyzing data from manufacturing processes.

Many of these resources are open to researchers in both academia and industry. In most cases, access is provided through a competitive peer-reviewed application process. In some cases, expedited access is provided for time-sensitive projects. Most of these resources require companies to pay for access or to keep their data private, which creates barriers to entry, especially for small companies and startups.

Programs to Connect Industry with Federal Resources and Experts

Various federal agencies have created programs to encourage collaboration with industry, many of which are applicable to the HEA community in industry.

The DOE HPC4Manufacturing[ab] **and HPC4Materials**[ac] **programs** provide access to the advanced computing capabilities at the DOE national laboratories based on proposals submitted by industry. The industrial partner identifys a manufacturing problem that could be solved using high-performance computing (HPC). Working with the industrial partner, experts at the national lab use the HPC assets at the lab to find a solution or set of solutions. Each partner (i.e., DOE and the industrial firm) pays for its own project-related costs.

The DOE Small Business Vouchers (SBV) program[ad] helps small businesses to access resources at the National Laboratories. The businesses recieve vouchers to offset the costs to interact with National Laboratories, which can be prohibitive. Currently implemented on a limited, pilot basis, the SBV program offers some opportunity for the HEA community to access the equipment and expertise of the National Laboratories to overcome technical barriers to commercialization.

The DOE Technologists in Residence program[ae] facilitates collaboration between industry and experts at the National Laboratories. Funded completely by DOE, the program allows industry and National Laboratory researchers to spend time at each other's facility to improve understanding of the challenges facing industry and the resources at the laboratories that can address those challenges.

y https://www.aps.anl.gov/
z https://www.energy.gov/eere/energy-materials-network/energy-materials-network
aa https://lift.technology/manufacturingusa/
ab https://hpc4mfg.llnl.gov/
ac https://hpc4mtls.llnl.gov/
ad https://www.sbv.org/
ae https://energy.gov/eere/cemi/technologist-residence-program

Applied to HEAs, these programs, combined with the other specific programs at various National Laboratories, could accelerate research, development, and commercialization. As examples such as CaloriCool and ElectroCat[af] illustrate, combining industry, academic, and federal laboratory facilities and expertise to define problems, structure an efficient problem-solving process, and focus resources on the most promising solutions is an effective mechanism for making rapid progress. These tools should be applied to HEAs.

Advisory Group

The consortium model is one promising approach to accelerating development and commercialization of HEAs across multiple applications. Consortia typically include joint R&D activities, funded collectively by the consortia members. The HEA community would also benefit from a few steps short of forming a consortium that would improve coordination of resource allocation and provide a mechanism to identify and focus on common precompetitive challenges. The recommended first step is to form an industry-wide Advisory Group.

An HEA Advisory Group should consist of members from industry (large, small, and start-up companies), academia, federal laboratories, and relevant federal agencies. Scientific and engineering expertise drawn from existing R&D efforts should be complemented by expertise from manufacturing, equipment suppliers, end users, and program managers. The group's objectives would be to provide a focal point for identifying and prioritizing technical challenges, market opportunities, and opportunities to support federal mission agencies while tracking research and development progress. Two specific tasks for the group are to create a roadmap to guide R&D efforts in the short, medium, and long timeframes, and to prioritize commercial opportunities based on effective analysis of a range of high-value applications, production costs, and the competitive environment.

HEA Manufacturing Roadmapping

HEAs span a broad range of materials and applications, which complicates efforts to achieve consensus on research and resource allocation. The same can be said about many nascent technologies. However, with appropriate participation of experts who clearly understand the possibilities and effective pathways to success, a roadmap to guide investments is both feasible and essential to move the field forward. The roadmapping effort should, at a minimum, address the following tasks:

1. Identify and assess the most promising and advanced (close-to-production) process technologies for scalability and applicability to different types of HEAs;
2. Match specific emerging manufacturing technology solutions with targeted application areas of national priority (e.g., defense, energy, and health) and interest; and
3. Develop long-term strategies to coordinate resources and accelerate innovation.

After developing the roadmap, the Advisory Group would track progress in meeting the roadmap objectives. The group would also work directly with the relevant researchers and industry participants to identify opportunities for industry to engage in early-stage research and to accelerate licensing and technology transfer to U.S.-based firms.

af http://www.electrocat.org/

Prioritization of Industry Needs

A key area to drive the switch from a technology push to an industry pull is the identification, prioritization, and communication of industry needs. Related efforts would include identification of applications, desired material property/performance suites, performance-driven specifications, specification boundary conditions, and technical challenges for scale-up. Existing federal programs, such as the Air Force Research Laboratory (AFRL) and the Department of Defense (DoD) ManTech[ag] and Office of Industrial Policy, can assist with identification in the defense and aerospace sectors.

Recommendation 4: Enhance collaborative efforts through increased access to existing federal facilities and expertise associated with advanced manufacturing methods, characterization tools, and computing power. In addition, establish an interdisciplinary working group to provide real-time input regarding manufacturing technology roadmapping, research priorities, standards, intellectual property, technology transfer, and other issues to facilitate accelerated progress.

ag https://www.dodmantech.com/


A Call to Action

HEAs are a rapidly expanding opportunity with cross-cutting applicability, serving as both a platform for economic growth and an essential technology to realize key national priorities from national security to health to energy efficiency. The United States has made significant investments in HEA research through a wide range of federal agencies and has developed world-class expertise and research facilities. Widespread utilization of HEAs, and a return on these investments, critically rely on advancing HEAs from lab-scale prototypes and simulations to products produced at scale by U.S. manufacturers.

The United States is well positioned to be the sustained global leader in HEA manufacturing, but targeted action must be taken quickly to realize and sustain this position. Acute challenges restrain HEAs from reaching their commercial potential and include manufacturing process know-how, modeling, high-throughput testing, centralized data activities, access to necessary equipment, and a lack of cohesion across the HEA community. Through coordinated action by stakeholders in academia, industry, and the federal government these barriers can be surmounted. From investments in translational research, to collaborations with federal facilities, to public-private partnerships, the federal government has a critical role to play.

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Appendix 2: Workshop Agenda (December 7, 2017)

Manufacturing High Entropy Alloys

8:00	Welcome and Introductions
8:30	Meeting Focus and Scope
8:45	Keynote: Dr. Dan Miracle, Air Force Research Lab
9:15	Break – proceed to Breakout Session 1

Identify Key Challenges to Scalable High Entropy Alloy Manufacturing

9:30	Session 1: Identification, Modeling, and Manufacturing Alloy discovery & development 1 Alloy discovery & development 2 Melting, casting, and forming Additive, powder, and emerging manufacturing
10:30	Break – proceed to Breakout Session 2
10:45	Session 2: Alloys and Applications High-temperature 1 High-temperature 2 Light-weighting Functional and emerging areas
11:45	Lunch
1:00	Report Outs and Group Discussion

Develop and Prioritize Actionable Recommendations

1:45	Overview of Actionable Recommendations
2:00	Sessions 3A-3D: Solutions and Recommendations
4:00	Break
4:15	Group Discussion of Key Actionable Items

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