# High Entropy Alloy Development for Fossil Energy Applications

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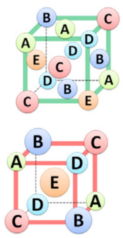
## INTRODUCTION

High-entropy alloys (HEAs) are loosely defined as solid solution alloys that contain five or more principal elements in equal or near equal atomic percent. The ideal configurational entropy of an equimolar solid solution increases with the logarithm of the total number of components in the alloy. HEAs and the more broadly-defined multi-principal-element alloys (MPEAs) represent a major paradigm shift in alloy design and are reported to have a combination of properties that include high strength, high toughness, and excellent creep, fatigue, wear, corrosion and irradiation resistance. These properties make them attractive for use in extreme environments. The high-entropy concept has now been extended from structural materials to ceramics, semiconductors, polymers, and a broad range of functional materials. However, configurational entropy does not always play a dominant role in materials properties. Four proposed core effects of HEAs including high entropy of mixing, severe lattice distortion, sluggish diffusion and cocktail effect have been theorized to play a role on materials performance.

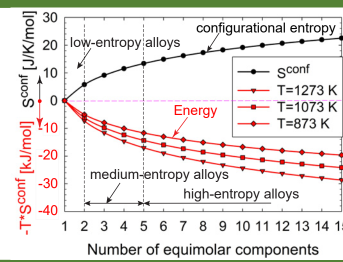


$$\Delta G_{mix} = \Delta H_{mix} - T\Delta S_{mix}$$

$$\Delta S_{mix}^{conf}\Big|_{ideal} = -R\sum_{i=1}^{N} x_i \ln x_i$$

$$\Delta S_{mix}^{conf}\Big|^{max} = RlnN$$

$$\Delta S_{mix} = \Delta S_{mix}^{conf} + \Delta S_{mix}^{el} + \Delta S_{mix}^{ph} + \Delta S_{mix}^{mag}$$



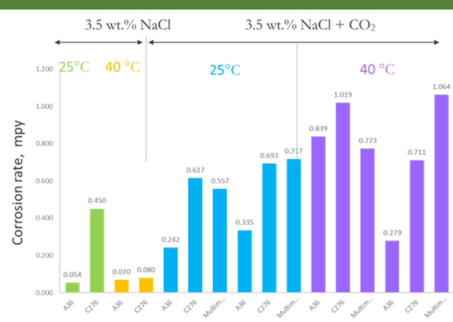

## NEED & APPROACH

Affordable, durable alloys for extreme environment service are needed to improve the effectiveness and efficiency of the existing fleet and enable advanced fossil energy systems. HEAs offer promise for severe service applications, due to the potential stability of these alloys at elevated temperatures relative to conventional alloys. The aim of this project was to design, manufacture, and evaluate HEAs for elevated temperature service and compared the results to conventional alloys and to explore extending HEA design concepts to improve the performance of conventional alloys for extreme environment service.

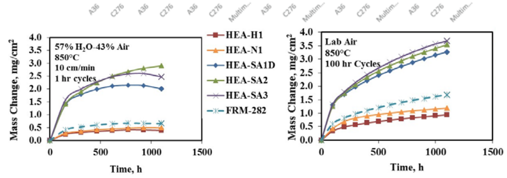
An integrated computational materials engineering (ICME) approach is used to accelerate design and development of high-performance structural materials. Multiscale computer modeling and simulations that bridge various length and time scales are used, including first-principles density functional theory (DFT), molecular dynamics, Monte Carlo, dislocation theory, calculation of phase diagrams (CALPHAD), and machine learning. Attention is paid to local atomic structures such as short range order that may impact mechanical properties. Guided by modeling and simulations, a variety of benchmark MPEAs (~7 kg – 15 lb) that were cast using vacuum induction melting followed by homogenization and thermo-mechanical processing. NETL alloys were produced as scales and methods that readily translate to industrial manufacturing. The microstructure, mechanical properties, oxidation behavior and aqueous corrosion were evaluated.

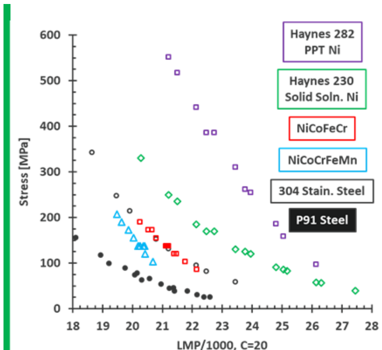
## RESULTS, BENEFITS, & FUTURE WORK

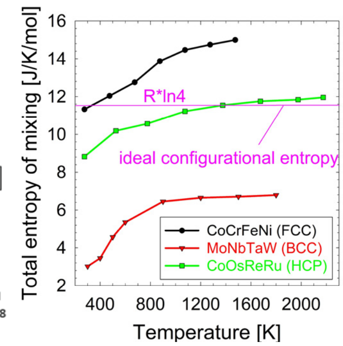
**NETL designed a corrosion resistant HEA (A36) based on CoCrFeNiMo. This is a single phase austenitic alloy. The performance was compared to Haynes Multimet and Hastelloy C276, commercial corrosion resistant alloys. NETL's A36 HEA performs as well or better than the commercial alloys in testing.**



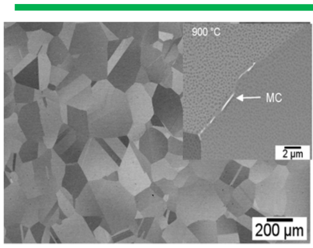

**The high temperature oxidation behavior of a FeNiCoCrMn single phase austenitic HEA. Test was done at 750 (not shown) and 850°C. The oxidation resists of NETL HEA-N1 and HEA-1N compare favorably to the commercial superalloy 282.**

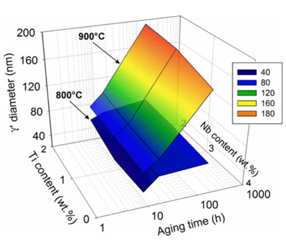


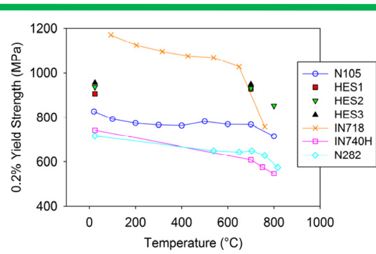




Computer modeling and simulations predict contributions from various entropy sources. Multiscale physics-based computer modeling and simulations coupled with machine learning will be implemented to predict short range order, intrinsic yield strength, and stacking faults energy of solid solution alloys.




**NETL applied HEA principles to re-design the matrix of gamma prime precipitation strengthened Ni-superalloys. The NETL High Entropy Superalloys (HEA) have good elevated temperature strength compared to conventional alloys used in advanced fossil energy power systems. Evaluation of the performance is continuing.**

Future work will be placed on further optimizing the microstructure (e.g., balancing the volume fractions of various phases ($\gamma$ matrix, $\gamma'$ precipitates, MC carbides, $M_{23}C_6$ carbides, and other strengthening precipitates) and thermo-mechanical processing (e.g., refining grain sizes, grain boundary engineering).

## ACKNOWLEDGEMENTS

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