High Entropy Alloys (HEAs): Properties, Comparative Analysis, and Engineering Applications.

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ABSTRACT- High Entropy Alloys or simply termed as HEA's are a major breakthrough in the field of material science showing properties which surpasses other materials used to a large extent. These types of alloys due to their high strength and immense light weight with a mix of thermal resistance is under consideration to replace previous game changer CFRP or Carbon Fiber. This study aims to deal with the overall science of physics and materials behind this alloy and how it stands among the plethora of existing materials along with major applications for which it is best suited. This study highlights the distinctive advantages inherent in HEAs, heralding transformative implications for industrial applications.

Keywords: High Entropy Alloys (HEA's), Material Science, Comparative Analysis, Lattice Structure, Thermodynamic Property, Entropy

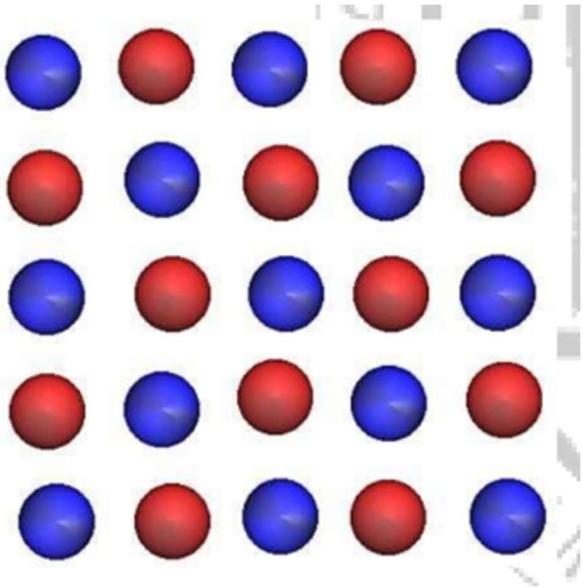
INTRODUCTION- Since the beginning of the world, mankind saw many phases of development in materials. We went from sharpening stones for hunting to turning wood logs for construction and at this age right now we are weaving fibers of carbon to get carbon fiber. Since the Bronze Age, alloys have traditionally been developed according to a 'base element' paradigm. This strategy begins with one and rarely two principal elements, such as iron in steels or nickel in superalloys, and a minor alloying approach is used to obtain alloys with enhanced properties. In sharp contrast, a novel paradigm for alloy design was proposed about a decade ago, which involves merely the mixing of multiple elements in an equimolar or near-equimolar composition to form alloys, thus eschewing the 'base element' concept (Y.F. Ye, 2016).

If we think outside the conventional box and design alloys not from one or two 'base' elements, but from multiple elements altogether, this new concept, first proposed in 1995 and has been named a high-entropy alloy (HEA) (Ming-Hung Tsai, 2014). HEAs can be defined as alloys with five or more principal elements. Besides the principal elements, HEAs can contain minor elements too, each providing a set of materialistic properties. These alloys are named 'HEAs' because their liquid or random solid solution states have significantly higher mixing entropies than those in conventional alloys. Thus, the effect of entropy is much more pronounced in HEAs. Existing physical metallurgy knowledge and binary/ternary phase diagrams suggest that such multi-element alloys may develop several dozen kinds of phases and intermetallic compounds, resulting in complex and brittle microstructures that are difficult to analyze and engineer, and probably have very limited practical value. In contrast to these expectations, experimental results show that the higher mixing entropy in these alloys facilitates the formation of solid solution phases with simple structures and thus reduces the number of phases. Such characters, made available by the higher entropy, are of paramount importance to the development and application of these alloys. Therefore, these alloys were named as 'high-entropy' alloys.

The high entropy can be simply explained as a higher degree of disorder between the subject here the alloy. Due to the composition of the elements that too in a large number that is near about 5 elements, the disorder or randomness is increased creating more entropy in the microstructure which lays as the paramount reason for this type of alloy. During the fabrication of HEAs there is very little need of special processing techniques or equipment, which indicates that the mass production of HEAs can be easily implemented with existing equipment and technologies. More than 30 elements have been used to prepare more than 300 reported HEAs, forming an exciting new field of metallic materials. This paper tends to provide a concise introduction to HEAs along with a clear-cut comparison of the alloy with

other popular materials used in engineering applications. For further understanding the paper proposes a theoretical approach to its promising application.

THE BACKGROUND- Before delving the alloy itself let's get over with the principal property of the alloy which is the name itself that is ENTROPY. **It** is a scientific concept that is most commonly associated with a state of disorder, randomness, or uncertainty in a thermodynamic system (Wehrl, 1978). There are many approaches in understanding entropy but for the sake of this paper and its main topic we will cover it with a material science aspect. The term is associated with the arrangement of molecules in the lattice arrangement a highly ordered lattice arrangement can be said to have negligible entropy while a disordered one may have higher entropy in it.

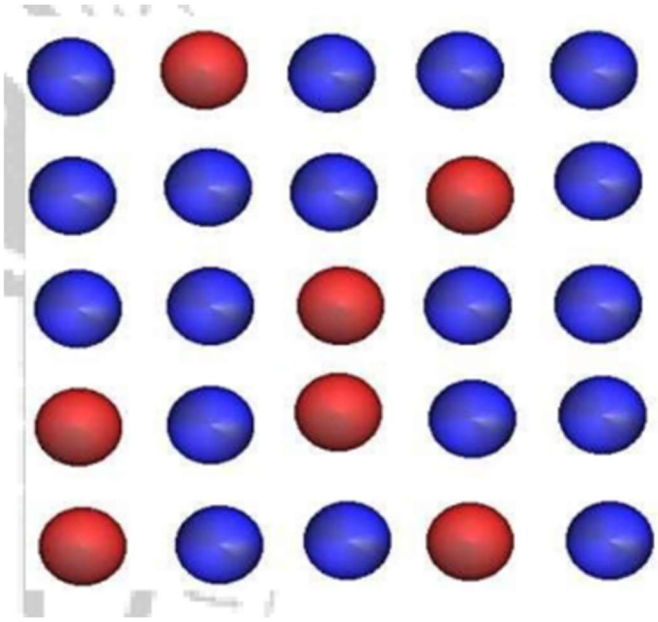


The figure above is a simplified representation of a regular ordered substitutional lattice arrangement of an alloy. The disorder or randomness is near to zero here as all the molecules of the alloy's elements are arranged in a format systematically. Here the entropy is very low and hence the arrangement tends to be weak due to presence of weak spots in the lattice structre.

The weak spots mentioned can be explained by taking an example, lets assume that the alloy is composed of 2 elements **(A)** and **(B)**. The element (A) in blue is tougher than (B) in red, and due to the ordered format of both element's molecules. (B)'s molecules are weak but essential as it exerts some vauable property so excluding it is not the option. Now when extreme stress or pressure is appied the material or the alloy will tend to fracture from the weak points of (B)'s molecules while the (A) will provide strength but due to the arrangement of (B) the material will fail.

This is the condition of normal materials used in the industry where the fracture occurs frequently and the resistance offered by the touger element is eventually gone to waste. The entropy here was low and due to this the fracture was quite evident and was not avoidable. The problem can be neglected by

taking an alloy with more random lattice arrangement produced pecifically for the applicatio and giving a much better result.



In the figure above the randomness is seen as the molecules are arranged more disoriented which gives rise to the property of entropy. The weakspots are there here too but more randomly placed which kind off increases the strength and thermal resistance. The entropy is defined well here as the lattice arrangement is too disordered along with random distribution of elements present.

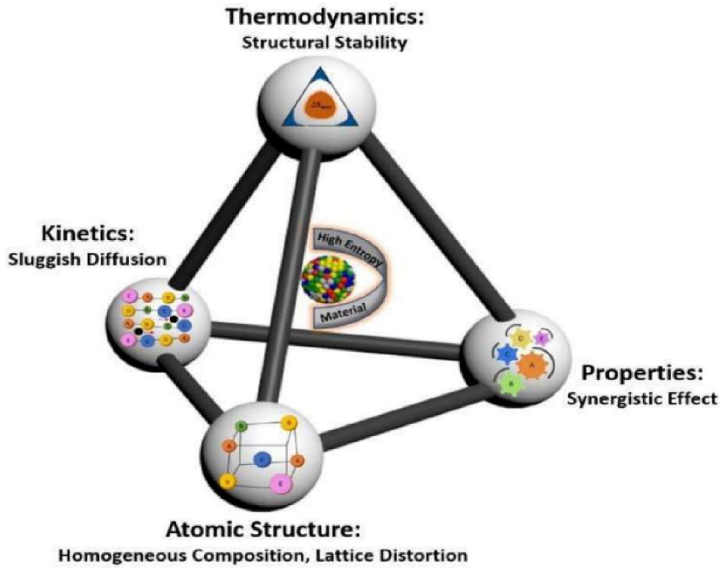
This diagram is not of HEAs but it is just for the explanation of why entropy is important and how it can be explained in diagrams as for material science.

THE FOUR CORE EFFECTS OF HEAs- Because of the multi-component composition, HEAs exhibit different basic effect than the other traditional alloys that are based only on one or two elements and these different effect are called "the four core effects of HEAs" (Yeh, 2013). These are the backbone behind a lot of
microstructural properties of HEAs along with electrical, mechanical and thermal properties. The four core effects are:

1) high-entropy:- it enhances the production of solid solutions and makes the microstructure much simpler and concise than expected. The prior knowledge expected to multi component alloys to have many different interactions among elements and thus form many different kinds of binary, ternary, and quaternary compounds and/or segregated phases. Thus, such alloys would possess complicated structure brittle by nature. This expectation in fact neglects the effect of high entropy effect (B. S. Murthy, 2019).

2) severe lattice distortion:- Because solid solution phases with multi-principal elements are usually found in HEAs and every atom is surrounded by different kinds of atoms and thus suffers lattice strain and stress mainly due to atomic size difference. Besides the atomic size difference,

both different bonding energy and crystal structure tendency among constituent elements are also believed to cause even higher lattice distortion because non-symmetrical bindings and electronic structure exist between an atom and its first neighbours. This distortion is believed to be the source of some of the mechanical, thermal, electrical, optical, and chemical behaviour of HEAs. Thus, overall lattice distortion would be more severe than that in traditional alloys in which most matrix atoms (or solvent atoms) have the same kind of atoms as their surroundings (O. N. Senkov, 2017)



Schematics of 4 core effects in HEAs (D. Mitrica, 2021)

3) Sluggish Defect:- an HEA mainly contains random solid solution and/or ordered solid solution. Their matrices could be regarded as whole-solute matrices. In HEAs, those whole-solute matrices diffusion vacancy are surrounded by different element atoms, and thus have a specific lattice potential energy (LPE). This large fluctuation of LPE between lattice sites leads to low-LPE sites can serve as traps and hinder atomic diffusion this leads to the sluggish diffusion effect.

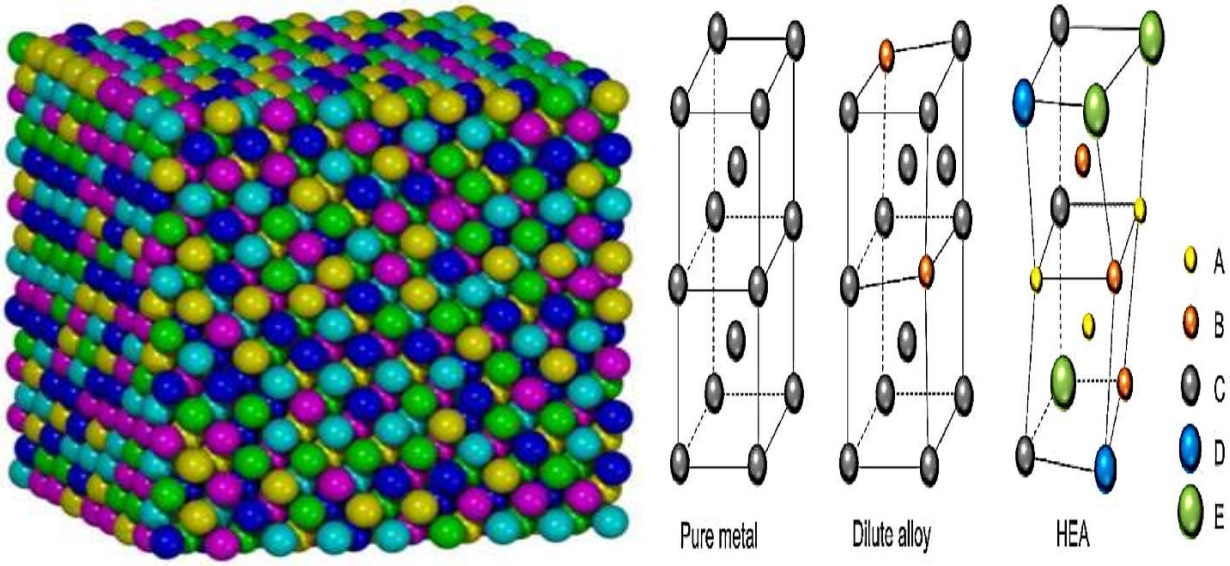
4) Cocktail effect:- is used to emphasise the enhancement of the properties by at least five major elements. Because HEAs might have one or more phases, the whole properties are from the overall contribution of the constituent phases. Besides, each phase is solid solution and can be viewed as a composite with properties coming not only from the basic properties of constituant by the mixture rule but also from the interactions among all the constituant and from the severe lattice distortion. The Cocktail effect take into account the effect from the atomic-scale multicomponent phases and from the multi phases composite at the micro scale (Xian, et al., 2018)

Atomic structure model of fcc CoCrFeMnNi consisting of Cobalt, Chromium, Iron, Manganese and Nickel which forms an High Energy Alloy with suitable entropy. The microstructure of equiatomic fcc CoCrFeMnNi high-entropy alloy (HEA) is characterized by a single-phase face-centered cubic (FCC) crystal lattice. This micro structure is a result of the high configurational entropy achieved by the near-equal mixing of the five constituent elements (Co, Cr, Fe, Mn, Ni). Unlike conventional alloys dominated

by a single element, the high entropy in CoCrFeMnNi disrupts the formation of ordered intermetallic compounds. Instead, the large atomic size difference between these elements favors a random solid solution, where the atoms of each element are distributed statistically throughout the FCC lattice.

This random distribution minimizes the Gibbs free energy of the system, promoting the formation of a single-phase structure. Transmission electron microscopy (TEM) analysis of CoCrFeMnNi HEA typically reveals a high density of dislocations within the FCC matrix (Ji, et al., 2015). These dislocations are a result of the rapid solidification processes often employed for HEA fabrication, such as arc melting or laser melting. The dislocations act as obstacles to slip during deformation, hindering dislocation movement and leading to a strengthening effect known as solid solution strengthening. This mechanism contributes significantly to the high strength and wear resistance observed in CoCrFeMnNi HEA.

Additionally, some studies have reported the presence of nanoscale twin boundaries within the microstructure. These planar defects can further enhance the mechanical properties by introducing additional barriers to dislocation motion and promoting a specific deformation mode known as twinning. The overall grain size of CoCrFeMnNi HEA is another crucial microstructural feature that can be influenced by processing parameters like annealing temperature and hot deformation. Finer grain sizes are generally associated with higher strength due to the Hall-Petch effect, which relates grain size to yield strength. Conversely, larger grains can improve ductility by allowing for more extensive dislocation movement before fracture. Therefore, controlling the grain size through thermo-mechanical processing becomes a tool for the mechanical properties of CoCrFeMnNi HEA to specific applications.

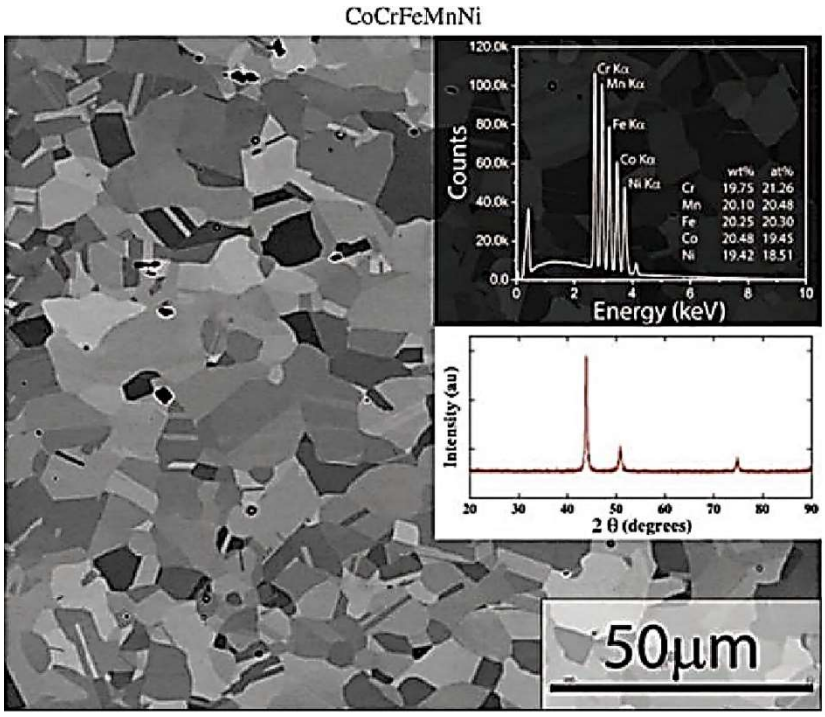


Lattice Structure of CoCrFeMnNi and HEA's (W. Li, 2021)

COMPARATIVE ANALYSIS- While materials like steel, iron, and aluminum have dominated for decades but the issue of low strength and lower thermal resistance is still evident which offers a great lag in production and performance issues. Whereas the HEAs offer a compelling alternative with unique properties. Following is a breakdown of how they compare:

1) **Strength and Toughness:** HEAs often outperform traditional materials in terms of strength and toughness. Their complex compositions create a "cocktail effect" where the different elements interact to hinder dislocation movement, leading to superior resistance to deformation and fracture. Imagine HEAs like a well-trained defensive line in football, effectively stopping any advance. (Ren, Shen, & Liu, 2013)

2) **High-Temperature Performance:** Traditional materials can weaken significantly at elevated temperatures. HEAs, however, boast impressive high-temperature stability. Their unique atomic arrangements reduce atomic mobility, a phenomenon known as "sluggish diffusion" (Zeng & Xu, 2020). This translates to excellent resistance to creep deformation at high temperatures, making them ideal for applications like jet engines and power plants, where things get hot and heavy (Middleburgh, King, Lumpkin, Cortie, & Edwards, 2014).

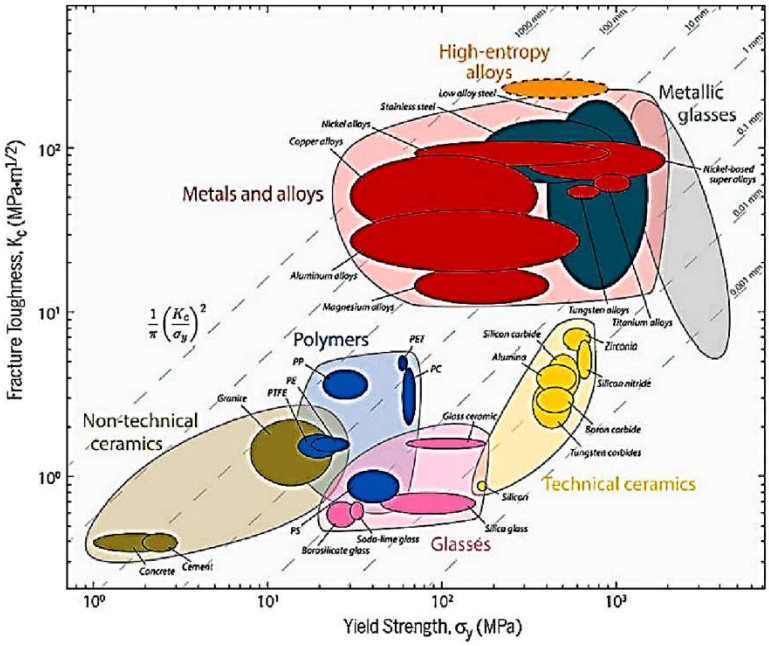


Microstructure of annealed CoCrFeMnNi alloy (B. Cantor, 2004)

3) **Tailoring for Specific Needs:** Traditional materials often come with a fixed set of properties. HEAs, with their vast compositional possibilities, offer a significant advantage. By adjusting the elements and their proportions, scientists can tailor HEAs to achieve specific properties for a particular application. Think of HEAs as a customizable suit of armor, designed to perfectly fit the needs of the situation (Troparevsky, 2015).

4) **Challenges and Considerations:** Despite their potential, HEAs are not without their drawbacks. Identifying optimal compositions for specific applications requires extensive research due to the vast number of potential combinations. Additionally, their complex nature often makes them trickier and more expensive to manufacture using conventional techniques [5]. Finally, HEAs are

a relatively new field, and the long-term behavior of these materials under various environmental conditions is still being explored (Lederer, Toher, Vecchio, & Curtarolo, 2018).



(B. Gludovatz, 2014)

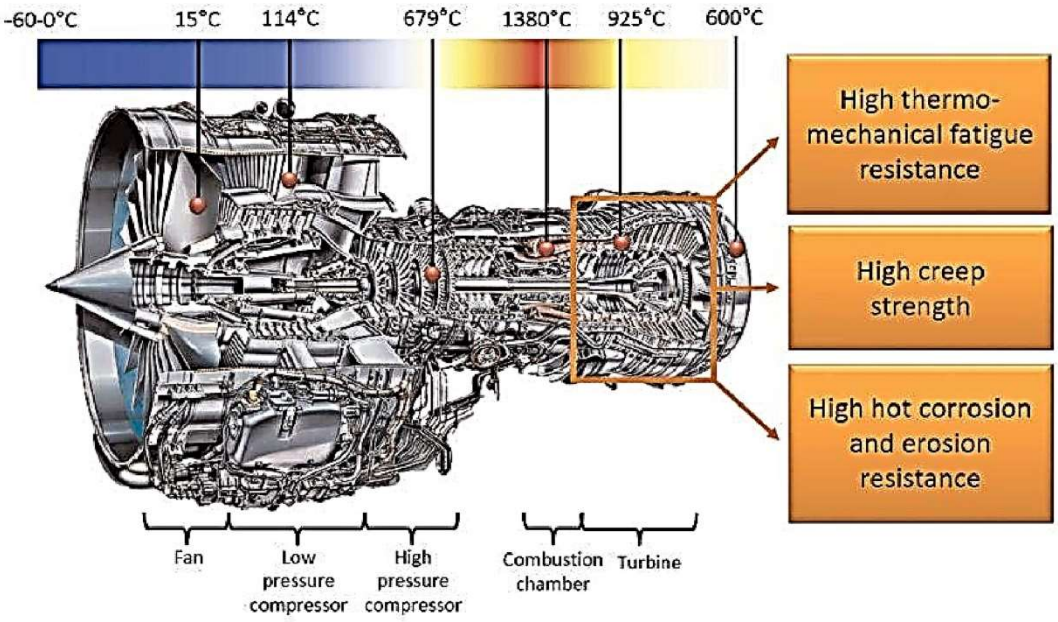
Comparison of fractural toughness & yielding strength of engineering materials with HEAs.

APPLICATIONS: HEAs are a promising replacement for utilization in the aerospace sector mainly in the production of jet engine, serving both structural and functional roles. These alloys offer enhanced microstructural stability across a wider temperature range, making them suitable for diverse operating conditions. Integration of HEAs with conventional alloy systems allows for concised solutions to meet the demanding requirements of complex engines. Welding and other manufacturing processes to be studied, it isessential for practical implementation, particularly for joining HEAs with nickel-based superalloys and stainless steel.

Innovations in welding technologies enable the fabrication of complex components, reducing the need for costly casting and machining operations. Weld repair techniques also contribute to extending service life and minimizing replacement costs. However, further research is needed to explore high temperature characteristics and heat treatment optimization of HEAs, as well as understanding the mechanisms underlying their strengthening properties.

The development of innovative materials for aeroengines that meet standards for thrust, weight, safety, fuel efficiency, life cycle costs, and environmental considerations has lately been challenged by competition from the aerospace sector. The development and implementation of structural materials that would provide higher performance and be more cost-effective to manufacture as well as repair than present components is required by contemporary current improvements and progression in the aeroengine sector. The ideal alloy that could withstand extreme temperatures and still be lightweight will be chosen based on the working environment. The material distribution of an aeroengine consists of

steels, titanium alloys, nickel superalloys, aluminum alloys, and more recently, HEAs. (Tushar Sonar, 2024)



The cross-sections of high temperatures in aeronautical jet engine (Mouritz, 2012)

HEAs offer promising attributes such as high strength-to-weight ratio, resistance to oxidation and fatigue, and thermal stability, making them suitable for critical components in aeroengines, including turbine blades, vanes, and combustion chamber's temperatures, stresses, and corrosive environments is crucial for progress in aeronautical science and technology. However, research in materials science requires careful planning due to its resource-intensive nature.

RESULTS & CONCLUSIONS:

- High-Entropy Alloys (HEAs) contain at least five major alloying elements within a specific atomic percentage range, exhibiting unique characteristics such as greater entropy and sluggish diffusion, setting them apart from traditional alloys.

- HEAs exhibit improved tensile characteristics compared to other materials, enhancing both strength and ductility. The structural arrangement, whether FCC- or BCC-structured, dictates the strength and plasticity of HEAs.

- Mechanical performance of HEAs remains exceptional across various temperatures, including ambient, cryogenic, and elevated, along with notable corrosion resistance and endurance limits.

- The diverse elemental composition and high mixing entropy of HEAs contribute to their mechanical superiority and enhanced strength-to-weight ratio, making them potential structural materials for engineering and aerospace applications.

- Heat treatment of the HEAs depending on composition and use, significantly influences the microstructural development and mechanical properties of HEAs, requiring optimization for desired characteristics, including considerations of duration, quenching medium, and heating/cooling rates.

- Research into the weldability and additive manufacturing of HEAs, both in similar and dissimilar configurations, is essential for their practical application in engineering.

- Theoretically fit for consideration of replacement in jet engine as in blade or exterior body component for elevated durability and resistance improving efficiency.

- HEAs present a promising option for structural and functional materials in aeroengines, capable of integration with conventional alloy systems to meet diverse operating demands.

Therefore, the paper dealt with overall background regarding the physics and mmaterials science behind the high entropy alloys along with the reason for their distinctive properties with comparative analysis. The study also highlighted and supported earlier results of integration of HEAs in aerospace jet engine for effeiency.

*** The information sourced from other studies are cited accoordingly with figures and representations. The claims and results are purely theroretical further study and experimentation is encouraged to the readers for obtaining the practical results.***

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