Final Year Project Showcase Batch-2021
Year 2025

Department: Metallurgical Engineering
Programme: Metallurgical Engineering

1 Project Idea

To predict the Mechanical Property (Y.S) of High Entropy Alloys (HEAs) via Machine Learning.

2 Process

A machine learning models is used to forecast the yield strength (Y.S) of High Entropy Alloys (HEAs) are the goal of this FYDP. The following standard ML procedure were used, which is indicated in the Fig. 1 flow diagram. Moreover, Streamlit End User Interface (EUI) was also developed to predict the Y.S, which is shown in the video link at the heading 9.

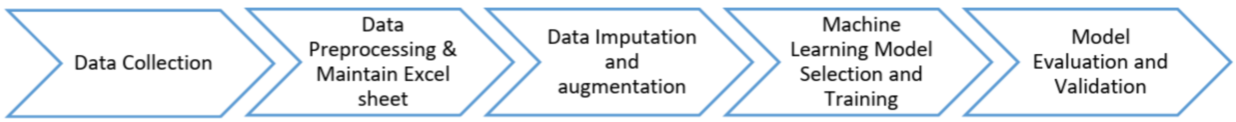

Fig.1: Process Flow Chart

3 Outcome

Created an interactive prediction tool using Python and Streamlit and demonstrated the feasibility of ML in Metallurgical design processes.

4 Evidence (Theoretical Basis)

The prediction of Mechanical Properties in High Entropy Alloys (HEAs) presents a significant challenge due to their vast compositional complexity and nonlinear structure–property relationships. HEAs consist of five or more principal elements in near-equiatomic ratios, giving rise to unique phenomena such as high entropy stabilization, severe lattice distortion, sluggish diffusion, and the cocktail effect. These features contribute to enhanced mechanical properties, but they also make experimental characterization time-consuming, material-intensive, and costly. Traditionally, determining the yield strength of an alloy requires physical experimentation, such as tensile testing, microstructural analysis, and phase characterization, all of which involve high energy input, costly laboratory equipment, and significant material usage. Furthermore, every new HEA composition necessitates repeated testing, contributing to resource wastage and increased environmental footprint.

To address this issue, the project introduces a machine learning–based framework that utilizes metallurgical theory and experimental datasets to predict the Mechanical Properties of HEAs without relying on extensive physical testing. The approach integrates the following and indicated in Fig.2: i. Elemental features (Al, Ti, Co, Si, Fe, Mn, etc.), ii.Physical properties (density), iii. Microstructural characteristics (phase type: FCC, BCC, mixed) and iv. Processing routes (casting, annealing, powder metallurgy)

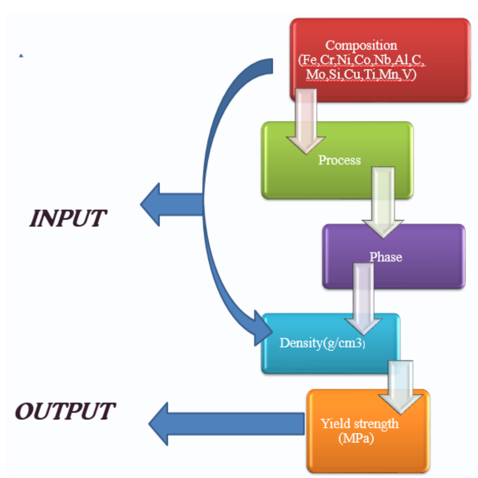

Fig.2: Flow Chart

These features are selected based on established principles in physical metallurgy and solid-solution strengthening mechanisms. Statistical models like Multilayer Perceptron (MLP), Support Vector Machine (SVM), and Back Propagation Neural Networks (BPNN) were trained on curated datasets extracted from published literature. The models were evaluated using R^2, RMSE, MAE, and MAPE, with MLP achieving the highest predictive accuracy (R^2 = 0.9919). The comparisons are shown in Fig. 3 and 4

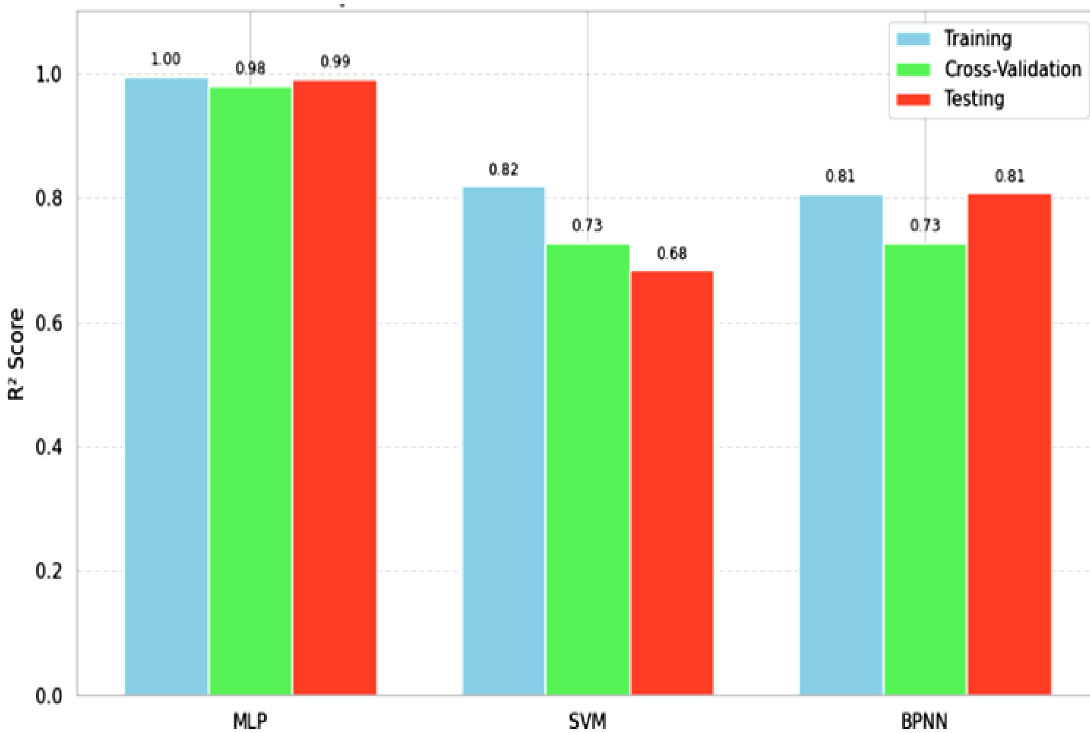

Fig. 3: Comparison of training, testing & validated R^2 value

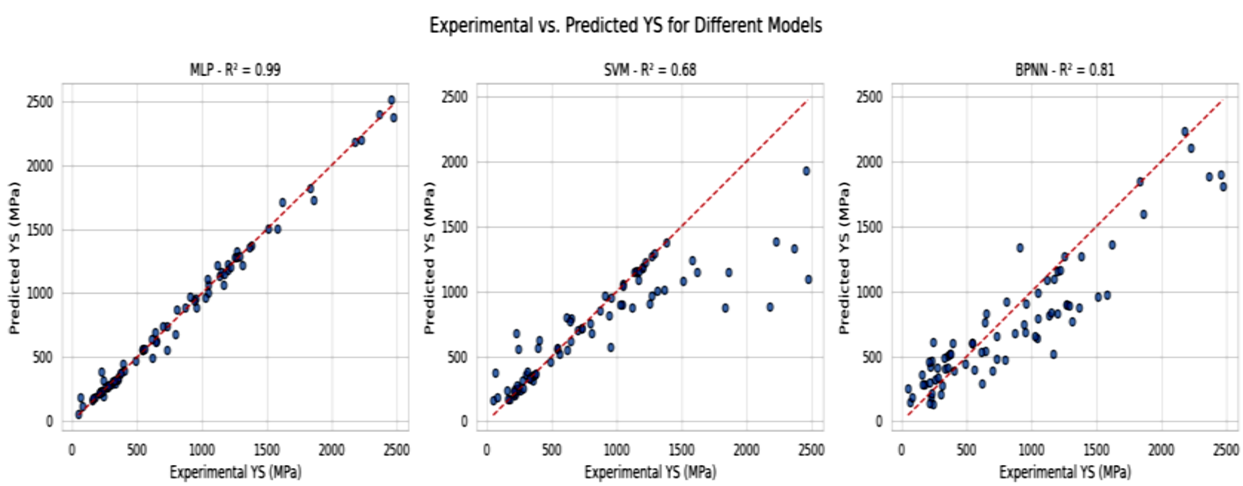

Fig. 4: MLP, SVM and BPNN Model showing experimental vs predicted Y.S.

The theoretical significance lies in the project's ability to capture complex non-linear relationships between input features and mechanical behavior, which are traditionally difficult to quantify through deterministic models alone. The relative significance of each input characteristic on the yield strength prediction using a Multi-Layer Perceptron (MLP) Regressor is shown in Fig.5.

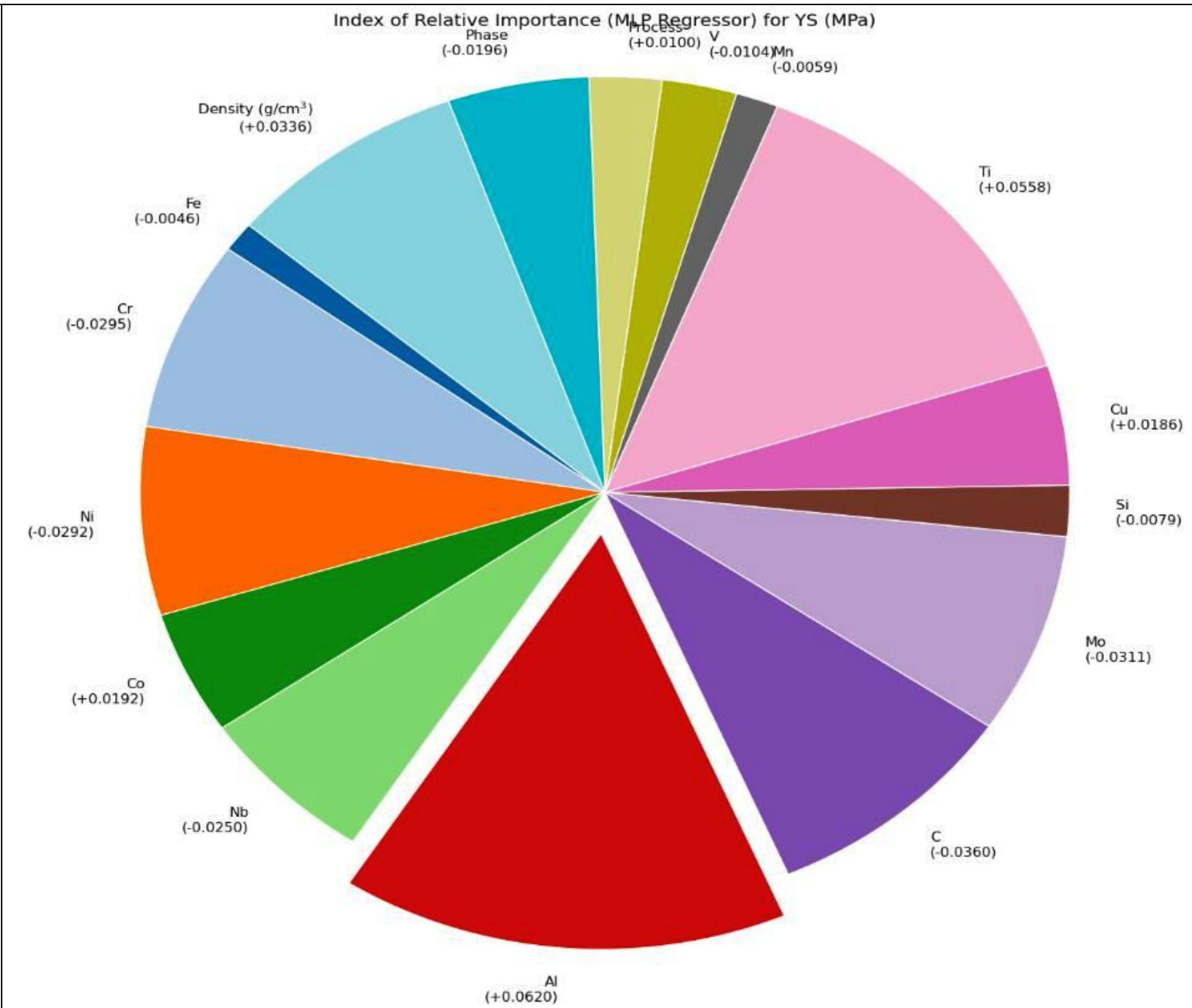

Fig. 5 Pie Cart MLP

The linear correlations between each element and the yield strength (YS), expressed in MPa, are shown in Fig 6. A color gradient from blue (negative correlation) to red (positive correlation) is used in the heatmap. Interestingly, aluminum (Al) and YS have a comparatively strong positive connection (r = 0.34), suggesting that aluminum has a strengthening influence on the alloy system. Conversely, there are negative associations between vanadium (V) and nickel (Ni), suggesting that larger concentrations of these metals may result in a decrease in YS. Denser alloys might also have lower yield strengths, as seen by the high negative correlation (-0.41) between density and YS. The choice of alloying elements for optimizing mechanical performance can be guided by this analysis.

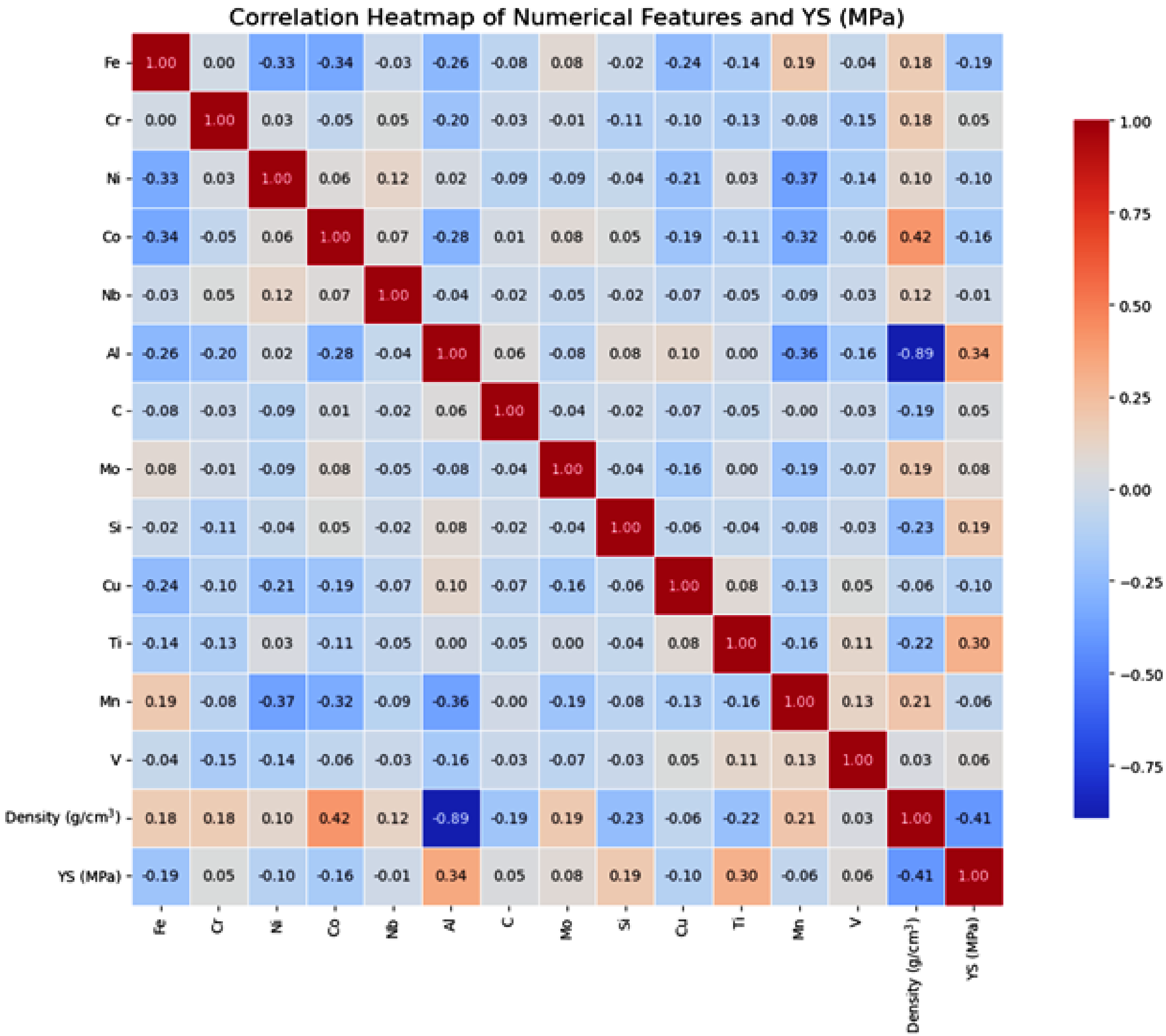

Fig. 6 Heat Map of MLP

The top five factors influencing yield strength, as determined by a permutation significance analysis, are displayed in the Fig 7. When a feature's values are randomly shuffled, this method calculates how much the model's predicted accuracy lowers; the larger the decline, the more significant the feature. The most important contribution, aluminum (Al), is by far the most substantial. Iron (Fe), silicon (Si), cobalt (Co), and titanium (Ti) are next in significance, albeit with less influence. These findings support the correlation study and highlight how important Al and Ti are to the material's strength. When creating high-strength alloys, the graph aids in prioritizing which factors to concentrate on.

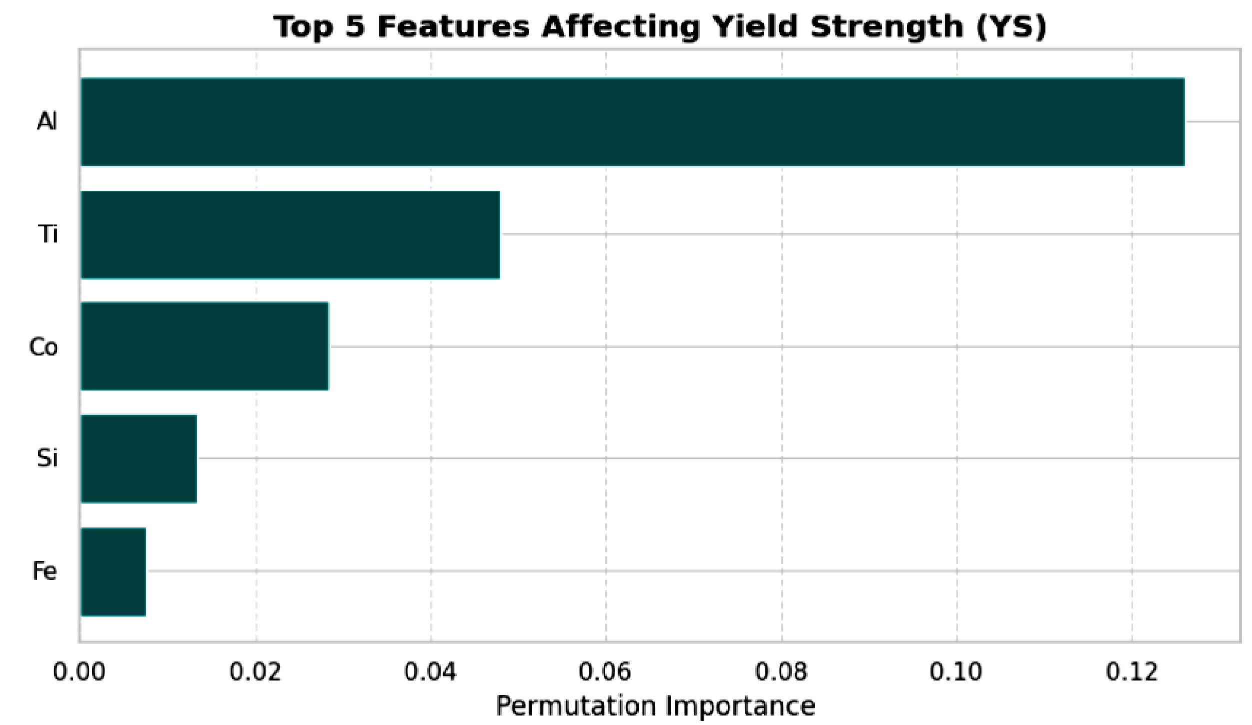

Fig 7. Top five feature importance- MLP

Yield Strength Prediction APP

This Streamlit APP predicts the Yield Strength (YS) of an HE-alloy based on user provided inputs. Users can enter the percentage of the elemental composition as Fe, Cr, Ni, Co, Nb, Al, C, Mo, Si, Cu, Ti, Mn, and V, along with density (g/cm^3), process type (e.g., CAST, WROUGHT), and phase (e.g., FCC, BCC). The video link at Heading 9 is provided herewith. After entering the required values, one can predict the estimated Yield strength (Mpa).

5

Competitive Advantage or Unique Selling Proposition

In this FYP work, the following aspects have been fulfilled:

A: Competitive Advantage:

i. The project delivers a competitive advantage by introducing a machine learning–based framework that enables accurate prediction of yield strength in High Entropy Alloys (HEAs), eliminating the need for extensive experimental testing.
ii. By training models on existing data and using features rooted in metallurgical theory (e.g., elemental composition, phase, density), it drastically reduces material usage, testing time, and cost, addressing major limitations in conventional alloy development.
iii. The use of models such as Multilayer Perceptron (MLP), which achieved R^2 = 0.9919, shows the accuracy and reliability of the digital process in real-world alloy design.
iv. A Streamlit-based prediction tool makes the technology accessible and scalable for industries, researchers, and students — empowering even non-experts to engage in advanced material selection.
v. This innovation provides industries with a faster, cleaner, and more intelligent pathway for alloy development — especially important for sectors likeaerospace, defense, nuclear, and advanced manufacturing.

B: Unique Selling Proposition (USP):

i. The project's USP lies in combining materials science with artificial intelligence to build a sustainable, intelligent method for alloy performance prediction — a capability that is still rarely implemented in Pakistan's industrial or academic landscape.
ii. Unlike traditional approaches that are resource- and time-intensive, this method enables virtual screening of new alloy compositions, allowing industries to explore multiple design possibilities without waste.
iii. The custom-built ML prediction tool provides real-time insights, helping engineers and

	researchers make informed decisions quickly, without relying solely on experimental setups. iv. The project promotes responsible consumption and production (SDG 12) by reducing material waste and encouraging data reuse through predictive analytics — a forward-thinking contribution to sustainable materials engineering. v. Its adaptability, accuracy, and environmental alignment make this project commercially viable and technically superior compared to conventional methods, giving it a distinct edge in competitive markets. The project's competitive advantage comes from its AI-powered, resource-efficient approach, while its USP lies in delivering a high-impact, sustainable solution for modern alloy design challenges. It's an ideal fit for industries seeking next-generation materials innovation with a focus on efficiency, accuracy, and environmental responsibility.
a	**Attainment of any SDG** (e.g. How it is achieved and why it is necessary for the region) **SDG 12: Responsible Consumption and Production** This project fulfills the aspect of "Attainment of an SDG," specifically SDG 12:Responsible Consumption and Production. Here's how it is achieved and why it is necessary for the region: Achievement of SDG 12: • The project aligns with SDG 12 by promoting resource-efficient practices in material design through the use of machine learning, which eliminates the need for excessive experimental testing and reduces material and energy waste. • It introduces an innovative, data-driven approach to predicting the yield strength of High Entropy Alloys (HEAs), supporting sustainable consumption of raw materials and minimizing production inefficiencies. • By integrating computational modeling and predictive tools, the project encourages a shift toward cleaner and smarter manufacturing processes, which are critical for achieving sustainable production patterns. • Additionally, the project fosters awareness and knowledge sharing in the field of sustainable materials development, enabling the adoption of low-waste practices across industrial and academic sectors in the region. Why it is necessary for the region: • Responsible consumption and production are essential for the region to minimize material waste and optimize resource usage in industrial practices, particularly in materials engineering and alloy development. • By using machine learning to predict yield strength of High Entropy Alloys (HEAs), this project significantly reduces reliance on costly and time-consuming experimental trials, resulting in less consumption of raw materials and laboratory resources. • The project enhances resource efficiency by enabling intelligent selection and design of materials, thereby supporting sustainable manufacturing and minimizing environmental impact. • Through the development of a predictive model and digital tool, the project encourages a shift toward data-driven, low-waste innovation in metallurgy—an approach that supports cleaner, smarter, and more sustainable production. In summary, the FYDP alignment with SDG 12 reflects its strong commitment to minimizing waste, maximizing efficiency, and promoting responsible material development, ultimately contributing to the region's sustainable industrial growth and environmental well-being.
b	**Any Environmental Aspect** Although the project does not directly measure environmental parameters like energy efficiency, it significantly contributes to environmental sustainability by reducing the need for repeated experimental testing. By leveraging machine learning models to predict yield strength, the project minimizes material wastage, labor-intensive processes, and excessive energy consumption, thereby indirectly supporting cleaner and more responsible production methods.

c	**Cost Reduction of Existing Product** This project reduces production costs by replacing extensive trial-and-error experimentation with a machine learning-based predictive approach. It promotes resource efficiency, saving both materials and time. The use of intelligent data analysis tools enables more accurate alloy design with fewer failed trials, lowering material and labor expenses. Additionally, knowledge sharing and digital tool development support capacity building, improving workforce efficiency and contributing to long-term, sustainable cost savings in materials engineering.
d	**Recommendations** For improvement in the process, the following measures are suggested; • **Expanded Datasets:** The model's capacity to generalize to new compositions will be improved by adding more experimental HEA data from various sources. • **Including Thermo-Physical Descriptors**: Characteristics such as valence electron concentration, atomic size difference, electronegativity difference, and enthalpy of mixing might enhance the model's physical interpretability. • **Advanced Learning Techniques:** To analyze complicated interactions in HEAs, future research may use explainable AI (XAI) techniques or deep learning architectures like CNNs or ensemble meta-learners. • **Real-World Integration**: In the future, these models may be used in alloy design processes to help materials scientists find and optimize HEAs with desired mechanical characteristics more quickly.
e	**Expanding of Market share**(e.g. how it expand and what is the problem with the current market The application of machine learning to predict the yield strength of High Entropy Alloys (HEAs) presents a transformative opportunity to expand their market share both locally and globally. HEAs offer exceptional mechanical properties, corrosion resistance, and thermal stability, making them ideal candidates for high-performance applications in aerospace, automotive, defense, nuclear, and energy sectors. However, their adoption in regions like Pakistan is limited due to high development costs, lack of awareness, and dependency on traditional alloy systems. Current Market Limitations: • Limited use of advanced AI-driven tools in local alloy development. • High experimental costs and time discourage HEA research by industries. • Lack of awareness among manufacturers, engineers, and policymakers about HEAs and their advantages. • Dependence on conventional materials (e.g., stainless steels, 7075 aluminum) due to familiarity and easier availability.
f	**Capture New Market** (e.g. Niche market or unaddressed segment) To capture new and niche markets through the development and prediction of High Entropy Alloys (HEAs)using machine learning, this project presents a data-driven pathway for advanced materials innovation that is currently underutilized in Pakistan. Traditional markets tend to rely on well-established alloys; however, emerging sectors increasingly demandcustomized, high-performance materialsthat conventional alloys cannot provide. Strategy to Enter New Markets: • Offer customized alloy design services using the ML model to meet specific mechanical or environmental requirements. • Collaborate with industrial R&D units, startups, and universities to co-develop solutions tailored for niche sectors. • Launch awareness campaigns, workshops, and technical demonstrations to educate potential users on the value and benefits of ML-driven HEAs. • Build partnerships with fabricators, material suppliers, and government research labs to ensure practical integration and trust.
6	**Target Market**(Industries, Groups, Individuals, Families, Students, etc) Please provide some detail

	about the end-user of the product, process, or service • **Aerospace Industry**: HEAs designed through predictive modeling are ideal for aircraft structural components, where high strength-to-weight ratio and durability are critical. • **Defense and Military Sector:** Demand for advanced armor materials, projectile-resistant surfaces, and high-performance components makes HEAs a strategic solution. • **Automotive and Transport:** Manufacturers seeking lightweight yet strong materials for electric vehicles, suspension systems, and engine parts benefit from predictive HEA design. • **Marine Engineering:** HEAs with enhanced corrosion resistance are suitable for offshore structures, naval vessels, and underwater equipment. • **Power Generation & Nuclear Industry:** Due to their ability to withstand radiation, high temperatures, and mechanical stress, HEAs are attractive in turbine blades, cladding materials, and reactor parts. • **Biomedical and Prosthetics Industry:** Specialized HEAs with biocompatibility and wear resistance are ideal for implants, surgical tools, and medical devices.	
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9	**Video (If any)**	https://drive.google.com/file/d/1hTO-myElhtDRs8Q1O2hcGz3QOfuuB4GH/view?usp=sharing