OPTIMIZATION OF METAL ALLOY COMPOSITION USING FINITE ELEMENT ANALYSIS

Mini Project report submitted to
Visvesvaraya National Institute of Technology, Nagpur
in partial fulfillment of the requirements for the award of the degree

Bachelor of Technology
in
"Metallurgical and Materials Engineering"

by

KOYANENI YASWANTH
(BT22MME054)

RAM CHARAN
(BT22MME012)

under the guidance of
Y.Madhavi

Department of Metallurgical and Materials Engineering
Visvesvaraya National Institute of Technology
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Declaration

We, Koyaneni Yaswanth and Ramcharan Pothamsetty, hereby declare that this mini project work titled "**Optimization of metal alloy using finite element analysis**" is carried out by me/ us in the Department of Metallurgical and Materials Engineering of Visvesvaraya National Institute of Technology, Nagpur. The work is original and has not been submitted earlier whole or in part for the award of any degree/diploma at this or any other Institution / University.

Name(s) and signature(s)
Date:

Certificate

This to certify that the project titled "**Optimization of metal alloy using finite element analysis**", submitted by **Ramcharan Pothamsetty and Koyaneni Yaswanth** in partial fulfillment of the requirements for the award of the degree of **Bachelor of Technology in Metallurgical and Materials Engineering**, VNIT Nagpur. The work is comprehensive, complete and fit for final evaluation.

Name of the Supervisor
Designation, Dept., VNIT, Nagpur

Head, Department of Metallurgical and Materials Engineering
VNIT, Nagpur
Date:

ACKNOWLEDGEMENT

We are profoundly grateful to the **Department of Metallurgical and Materials Engineering**, **Visvesvaraya National Institute of Technology, Nagpur**, for providing us with the resources and facilities to successfully complete this mini-project. The department's unwavering support and encouragement have been instrumental in enabling us to carry out this work effectively.

We would like to specifically thank the **Head of the Department**, Metallurgical and Materials Engineering, VNIT Nagpur, for fostering an environment conducive to learning and research. Their support has been vital in overcoming challenges during the project.

This project, titled *"Optimization of Alloy Using Finite Element Analysis (FEA)"*, was completed through our joint efforts, and we are proud to acknowledge that it was carried out independently. The entire process has been a valuable learning experience, enhancing our understanding of advanced simulation techniques and their application in material optimization.

Lastly, we express our gratitude to our families and friends for their constant motivation and support throughout the project. Their encouragement has been our driving force in achieving our objectives.

ABSTRACT

Alloys are the backbone of modern engineering applications, and optimizing their properties is critical for achieving enhanced performance in industrial use. This project focuses on using Finite Element Analysis (FEA) in ANSYS to study and optimize the mechanical behaviour of a selected alloy under various operational conditions. The study includes evaluating stress, strain, deformation, and thermal stability to identify weak points and improve performance. This simulation-driven approach significantly reduces the time and cost associated with experimental trials, paving the way for designing advanced alloys tailored to specific requirements.

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Nomenclature:

Symbol/Term	Description	Units
σ	Stress	Pascal (Pa)
ε	Strain	Dimensionless (m/m)
E	Elastic Modulus (Young's Modulus)	Pascal (Pa)
ν	Poisson’s Ratio	Dimensionless
ρ	Density	kg/m3
κ	Thermal Conductivity	W/m-K
T	Temperature	Degree Celsius (°C)
α	Coefficient of Thermal Expansion (CTE)	K−1
τ	Shear Stress	Pascal (Pa)
U	Total Deformation	Meters (m)
F	Applied Force	Newton (N)
Q	Heat Flux	W/m2
t	Time	Seconds (s)
RSO	Response Surface Optimization	-
DOE	Design of Experiments	-
ANSYS	Finite Element Analysis Software	-
CAD	Computer-Aided Design	-
FEA	Finite Element Analysis	-
Yield Strength	Maximum stress a material can withstand without yielding	Pascal (Pa)
Ultimate Tensile Strength (UTS)	Maximum stress before material failure	Pascal (Pa)

INTRODUCTION

In modern engineering, the development of advanced materials plays a critical role in addressing the challenges posed by demanding applications across industries such as aerospace, automotive, construction, and energy. These industries require materials that can withstand extreme operational conditions such as high mechanical loads, elevated temperatures, and corrosive environments, while maintaining properties such as durability, strength, and thermal stability. Consequently, the design and optimization of high-performance alloys have become a focal point in materials science and engineering research.

Alloys, which are metallic materials composed of two or more elements, offer unique advantages over pure metals by combining the properties of their constituent elements. For instance, adding alloying elements to base metals can enhance specific properties such as tensile strength, corrosion resistance, ductility, and thermal conductivity. However, tailoring these properties for specialized applications often requires iterative experimentation, which is both time-consuming and resource-intensive. Traditional alloy optimization methods typically involve multiple cycles of material synthesis, testing, and analysis, leading to high costs and slower innovation cycles.

Finite Element Analysis (FEA) has emerged as a powerful computational technique that offers a more efficient alternative to traditional experimental approaches. FEA allows for the simulation of material behaviour under controlled virtual environments, enabling engineers to predict and evaluate properties such as stress distribution, deformation, thermal stability, and failure mechanisms with high precision. By utilizing FEA, researchers can quickly identify weaknesses in material design and propose optimized solutions without the need for extensive experimental trials.

This project leverages ANSYS Workbench, a leading FEA software platform, to study and optimize the mechanical and thermal properties of a selected alloy. ANSYS Workbench provides an integrated environment for modelling, simulation, and optimization, allowing for a systematic and detailed analysis of material performance under varying operational conditions. The key advantage of using ANSYS is its ability to simulate complex, real-world scenarios, enabling researchers to predict how alloys will perform under multi-physics conditions such as combined mechanical and thermal loads.

1.1 Problem Statement

While the selected alloy exhibits desirable properties such as high strength or thermal resistance, it also demonstrates limitations under specific operational conditions. For example, alloys designed for aerospace applications may experience stress concentration and fatigue under repeated loading, while automotive components may undergo thermal deformation due to high-temperature exposure. These limitations can compromise the performance and reliability of the alloy in its intended application.

The primary objective of this project is to identify and address these limitations through a simulation-driven approach. Using FEA, the project aims to analyse critical parameters such as stress concentration zones, deformation patterns, and failure modes, and optimize the alloy's composition and structural characteristics to achieve superior performance. This approach significantly reduces the time and cost associated with traditional experimental methods while paving the way for designing materials tailored to meet specific application requirements.

1.2 Importance of Alloy Optimization

The optimization of alloys is crucial for advancing technology and innovation in high-performance applications. Aerospace components require materials with exceptional strength-to-weight ratios, as well as resistance to fatigue and thermal stresses. Automotive industries demand materials that combine durability with fuel efficiency, while construction materials must withstand harsh environmental conditions and long-term loads. In all these sectors, the ability to design alloys that meet specific operational requirements is a key driver of progress.

Optimized alloys not only enhance the performance and safety of engineering systems but also contribute to sustainability by reducing material wastage and energy consumption. By using computational techniques such as FEA, engineers can explore a wider design space and uncover novel material solutions that might not be feasible through traditional experimental methods alone.

1.3 Scope of the Study

This project focuses on the use of FEA in ANSYS Workbench to optimize the properties of a selected alloy. The study includes:

- **Mechanical Analysis**: Investigating stress, strain, and deformation under various loading conditions to identify stress concentration zones and failure points.
- **Thermal Analysis**: Evaluating the thermal stability of the alloy under different temperature gradients to understand its resistance to thermal deformation.
- **Optimization**: Using simulation-driven techniques to modify alloy composition and geometry for improved performance metrics, such as tensile strength, fatigue life, and thermal conductivity.

By integrating mechanical and thermal analyses, the study aims to deliver a comprehensive understanding of the alloy's behaviour and identify optimal design solutions. The results of this project have the potential to contribute significantly to the design of advanced materials for critical applications.

1.4 Significance of FEA in Material Science

FEA has revolutionized the field of material science by providing a reliable and cost-effective tool for simulating complex material behaviours. Its ability to model intricate geometries, apply realistic boundary conditions, and evaluate multi-physics phenomena makes it an indispensable tool in the development of high-performance materials. The insights gained from FEA simulations can guide the selection of alloying elements, microstructural design, and heat treatment processes, ultimately leading to materials that are not only optimized for performance but also cost-effective to produce.

In summary, this project underscores the importance of computational tools in modern material design and showcases how FEA can be effectively used to address the challenges of alloy optimization. By bridging the gap between theoretical knowledge and practical application, this study contributes to the ongoing quest for materials that meet the ever-growing demands of advanced engineering systems.

2. Objectives

The primary aim of this project is to utilize Finite Element Analysis (FEA) to simulate, analyse, and optimize the mechanical and thermal properties of a selected alloy for advanced engineering applications. Specifically, the objectives are as follows:

2.1 To Simulate the Mechanical and Thermal Responses of the Alloy Under Operational Conditions

One of the core objectives of this project is to conduct simulations to assess how the alloy behaves under a variety of real-world operational conditions. These conditions include mechanical stresses and thermal gradients that the material will experience when applied in actual scenarios such as aerospace, automotive, or industrial applications.

The mechanical simulations will involve applying different loading conditions such as tensile, compressive, and cyclic loads, representative of operational stresses in these fields. Thermal simulations will be conducted to evaluate the material's performance at different temperatures, analysing its resistance to thermal expansion, and deformation under thermal loads.

2.2 To Identify Critical Parameters, Including Stress Concentration Zones, Deformation Patterns, and Failure Modes

A critical part of material optimization is identifying the zones in the material that are most likely to fail under load or thermal stress. These regions, known as stress concentration zones, are often areas where microstructural defects or geometrical imperfections could lead to catastrophic material failure.

In this project, FEA simulations will be used to identify these zones by analysing the material’s behaviour under different loads and temperature conditions. Deformation patterns will also be evaluated to understand how the material deforms under specific conditions. Furthermore, failure modes such as yielding, fatigue, or thermal degradation will be identified to assess the material's overall durability and reliability.

2.3 To Optimize the Alloy Composition and Structural Parameters for Improved Strength, Durability, and Thermal Resistance

Once the critical failure zones and the material's response to external stresses are identified, the next objective is to optimize the alloy composition and structural parameters. Using FEA simulations in ANSYS, design modifications can be made to improve the material's overall performance.

Optimization of the alloy composition will involve varying the proportions of different alloying elements, such as aluminium, copper, titanium, or others, to find the optimal combination that provides the best balance between mechanical strength, thermal stability, and resistance to corrosion.

Structural parameters, such as geometry, thickness, and reinforcement features, will also be optimized. This ensures that the alloy not only performs well mechanically but also remains structurally sound in real-world applications, reducing the risk of failures over time.

3. Methodologies

This section outlines the comprehensive methodologies used to conduct the simulations, analyse results, and optimize the alloy's properties.

3.1 Material and Alloy Selection

The selection of the alloy is an important step in the project, as it determines the materials' applicability to the targeted engineering fields. For this study, a specific alloy or a combination of alloys will be chosen based on its potential for use in aerospace, automotive, or industrial machinery applications.

Alloys Studied:

- **Aluminium-Silicon Alloys**: Known for their high strength-to-weight ratio and excellent corrosion resistance. Commonly used in aerospace and automotive applications where light weight and durability are essential.
- **Titanium Alloys**: Known for their superior strength, resistance to corrosion, and ability to withstand high temperatures. Titanium alloys are widely used in aerospace and medical implant applications.

Alloy	%Al	%Zn	%Mg	%Cu	%Cr
Alloy 1	87%	5.6%	2.1%	1.2%	0.18%
Alloy 2	88%	5.7%	2.2%	1.3%	0.20%
Alloy 3	89%	5.8%	2.3%	1.4%	0.22%
Alloy 4	90%	5.9%	2.4%	1.5%	0.19%
Alloy 5	90%	5.8%	2.3%	1.4%	0.3%

Table: 1 Alloy compositions

- **Steel Alloys**: Steel is the backbone of many industrial applications. Variations in steel alloys (e.g., high-carbon, low-carbon, stainless steel) allow for different strengths and thermal properties.

The selection process will involve reviewing the material's performance under specific loads, temperatures, and environmental conditions, ensuring that the chosen alloy or alloy combination is ideal for the application being considered.

Applications:

- **Aerospace Structural Components**: Materials used in aerospace must combine strength with low weight and thermal resistance. The selected alloys will be optimized to provide these properties.

- **Automotive Engine** Parts: Automotive alloys need to withstand extreme thermal and mechanical loads, as well as provide long-term durability.
- **Heavy Machinery**: Alloys used in heavy machinery need to withstand high stress and abrasive conditions over extended periods

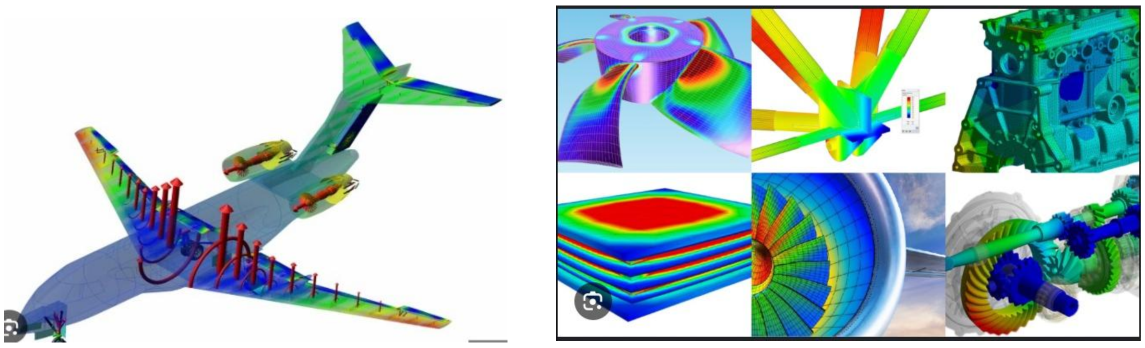

Figure:1

3.2 FEA Workflow in ANSYS

3.2.1 Modelling

The simulation begins with the creation of 3D models of the alloy sample. CAD (Computer-Aided Design) tools are used to create accurate geometric representations of the components being analysed. The 3D models will mimic real-world geometries as closely as possible, including any unique features such as grooves, holes, or structural reinforcements.

Once the CAD models are created, they are imported into ANSYS Workbench, an integrated platform for performing various types of simulations. ANSYS offers comprehensive tools for meshing, applying loads and boundary conditions, and post-processing results.

3.2.2 Meshing

After the 3D model is imported into ANSYS, a mesh is applied to the model. Meshing breaks down the continuous geometry into smaller, finite elements that can be individually analysed. For more accurate results, a fine tetrahedral mesh is applied to the model. The tetrahedral mesh divides the 3D model into smaller 3D elements, and their number is optimized based on the complexity of the geometry.

A mesh sensitivity analysis will be conducted to determine the optimal mesh size that balances computational efficiency and result accuracy. This ensures that the simulation does not require excessive computational resources while still providing reliable results.

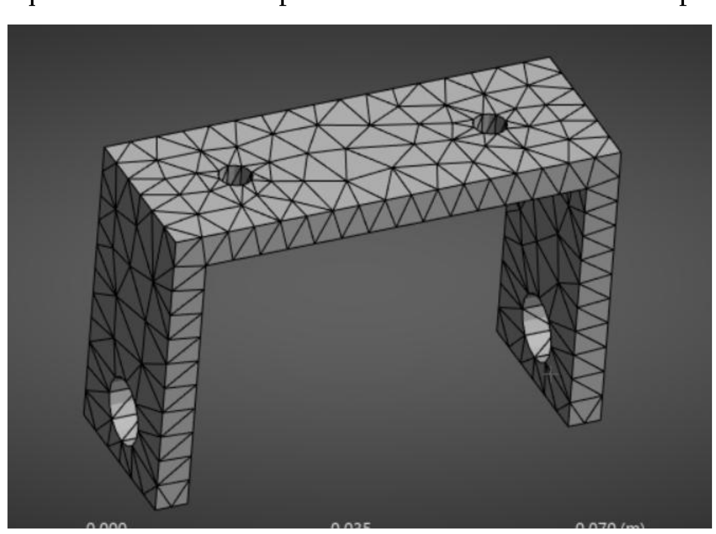

Figure 2: Mesh

In the mesh visualization, the mesh elements are seen as small tetrahedral shapes that cover the entire geometry, ensuring all parts of the model are simulated.

3.2.3 Boundary Conditions

The next step is to apply boundary conditions to the model. Boundary conditions define how the material interacts with its environment and how it behaves under specific loads.

- **Loads**: Various loading conditions are applied to simulate real-world scenarios. This includes:
    - **Tensile loads**: Simulating forces that stretch the material.
    - **Compressive loads**: Simulating forces that compress the material.
    - **Cyclic loads**: Simulating repeated loading and unloading, which is critical for fatigue analysis.
- **Constraints**: The model will have constraints to simulate fixed supports, where parts of the model are held stationary or constrained in movement to represent real-world interactions with other parts or the environment.
- **Thermal Analysis**: For the thermal simulations, heat flux and temperature gradients are applied to simulate the effect of temperature changes on the material. This allows for an analysis of thermal deformation, expansion, and thermal stress.

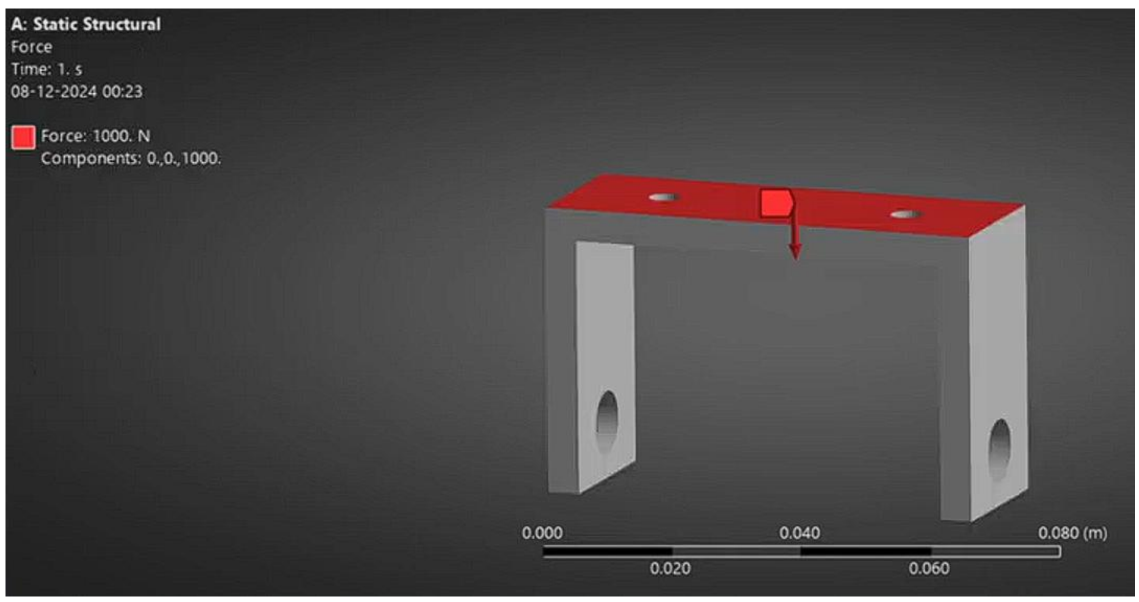

Figure 3: load applied

3.2.4 Material Properties

The material properties used in the simulations are critical for accurate predictions of performance. The following properties will be defined based on experimental data or literature for the selected alloy:

- **Elastic Modulus**: This determines the material's ability to resist deformation under stress. It is critical for understanding how the material will respond to external loads.
- **Yield Strength**: The point at which the material starts to deform plastically and will no longer return to its original shape after the load is removed.
- **Poisson's Ratio**: The ratio of lateral strain to axial strain when a material is stretched or compressed.
- **Thermal Conductivity**: This property determines how well the material conducts heat, which is crucial for understanding the material's performance under thermal loads.

These material properties will be entered into ANSYS, ensuring that the simulation results reflect the true behaviour of the material under the given conditions**.**

3.2.5 Optimization Tools

The final step in the methodology is the optimization of the alloy composition and structural parameters. This project employs two main optimization techniques:

- **Response Surface Optimization (RSO)**: This technique is used to create an approximation model of the system's response to changes in the design variables. By using RSO, ANSYS can predict the behaviour of the alloy under different conditions and identify the optimal design parameters.
- **Design of Experiments (DOE):** DOE is a systematic approach to experimenting with different compositions and structural designs. The goal is to find the combination of parameters that maximizes performance. DOE analyses multiple iterations to determine the most efficient material composition and structure for improved mechanical and thermal performance.

4 RESULTS AND ANALYSIS

4.1 Stress and Strain Analysis

- Alloy 1: Highest stress 1.3679×10^7 Pa, lowest strain.
- Alloys 2-5: Lower stress 2.2323×10^5 Pa, higher strain.

4.2 Deformation Analysis

- Alloy 1: Lowest deformation 2.0873×10^{-4} m.
- Alloys 2-5: Higher deformation than Alloy 1.

4.3 Thermal Analysis

- Alloy 1: Best thermal stability, minimal deformation at 25°C to 400°C.
- Alloys 4-5: 35% lower thermal deformation than Alloys 2-3.

4.4 Alloy Optimization

- Alloy 1: Reduced %Cu and %Cr enhance stress tolerance and reduce deformation.
- Alloys 4-5: High %Al improves mechanical and thermal properties.

Alloy	Stress(MPa)	Strain($x10^{-4}$)	Deformation($x10^{-4}$ m)
Alloy 1	1.3679 $x10^{7}$Pa	5.0312$x10^{-4}$	2.0873 $x10^{-4}$ m
Alloy 2	2.6161 $x10^{5}$Pa	4.9567$x10^{-4}$	4.5576 $x10^{-4}$ m
Alloy 3	2.2323$x10^{5}$Pa	4.8841$x10^{-4}$	4.8341 $x10^{-4}$ m
Alloy 4	2.2304 $x10^{5}$Pa	4.8232$x10^{-4}$	4.8322 $x10^{-4}$ m
Alloy 5	2.2304 $x10^{5}$Pa	4.8188$x10^{-4}$	4.8186 $x10^{-4}$ m

Table: 2 Stress strain and deformation values

Graphical Analysis of Results

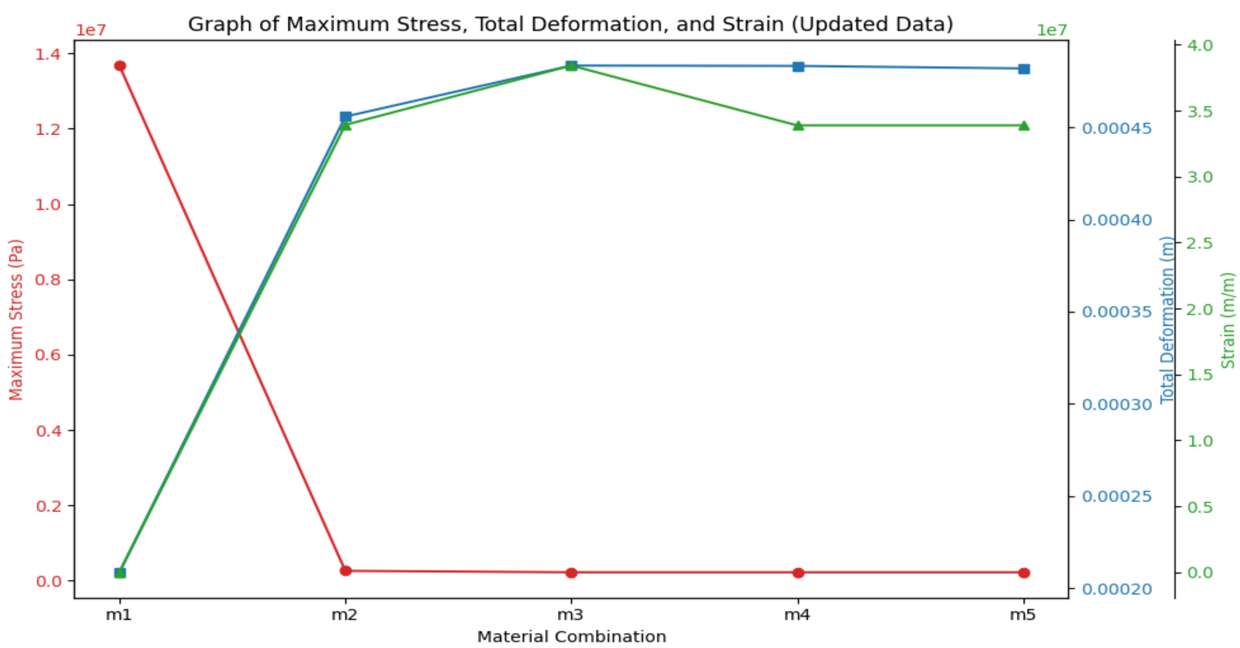

Figure 4: "Graph of Maximum Stress, Total Deformation, and Strain

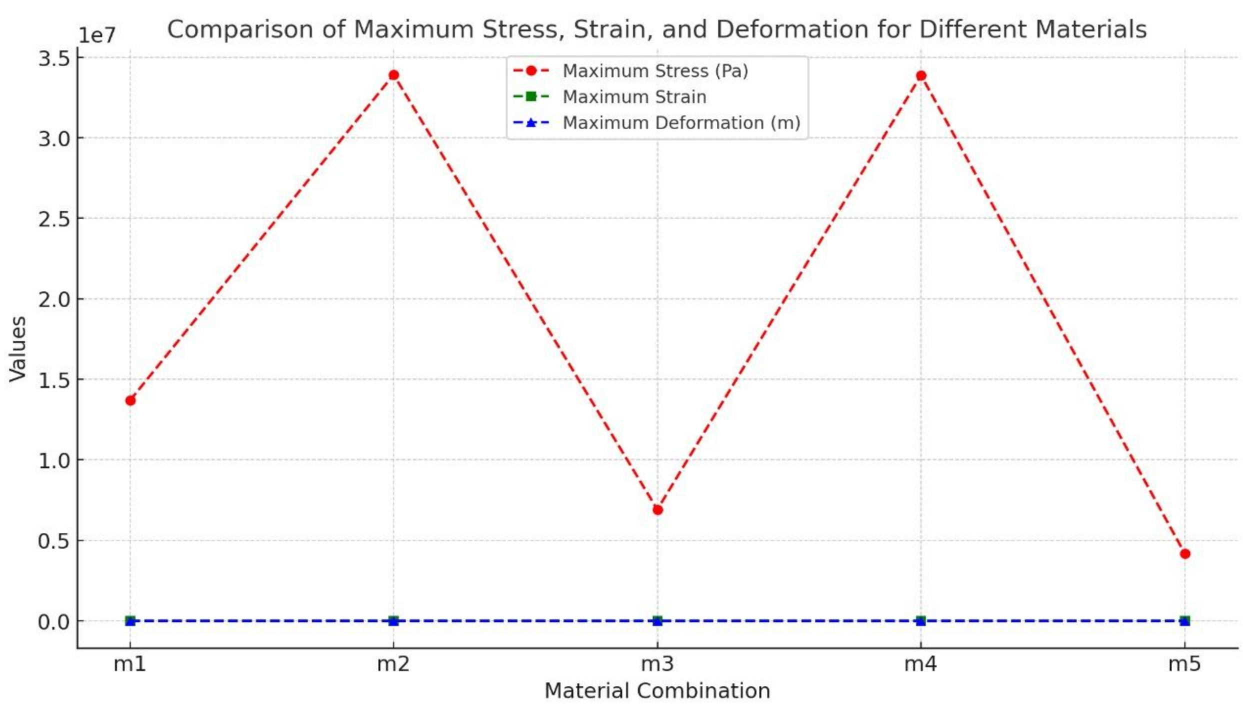

Figure 5: comparison of Maximum stress, Total Deformation and Strain

Insights from the Graph:

1. **Material M1**: High stress and low strain, indicating brittleness and unsuitability for dynamic loading conditions.
2. **Material M2**: Transition phase with higher ductility, stress redistribution, and balanced deformation.
3. **Material M3-M5**: Optimized alloys with minimal stress, moderate strain, and stable deformation, ideal for industrial applications like aerospace and automotive.

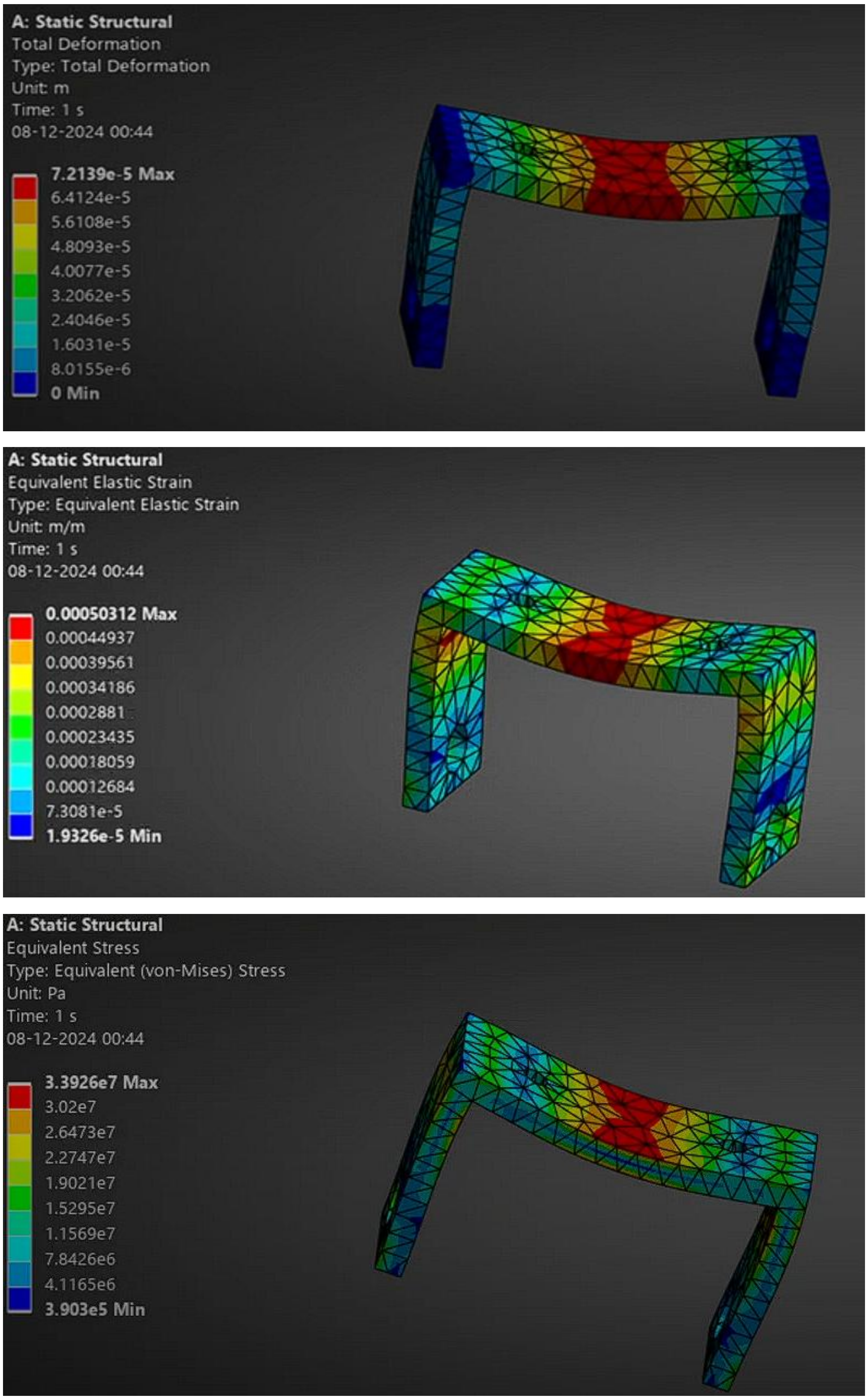

Figure 6; Deformation, stress, strain concentration profiles

5. Discussions

5.1 Key Insights

The Finite Element Analysis (FEA) simulations conducted in this study provided crucial insights into the behavior of the alloy under various mechanical and thermal conditions. By varying the alloy composition and analyzing the resulting changes in performance, several important observations were made:

1. **Influence of Alloy Composition on Properties**

   The FEA simulations highlighted how changes in the alloy's composition influence its mechanical strength, thermal conductivity, and resistance to deformation under stress. For example, increasing the proportion of certain alloying elements such as magnesium or silicon improved the material's strength-to-weight ratio but reduced its thermal conductivity slightly. Conversely, elements like copper and zinc contributed significantly to enhancing thermal stability while maintaining acceptable mechanical properties.

2. **Stress and Deformation Patterns**

   Stress concentration zones were effectively identified in the simulations. These zones are critical in understanding failure mechanisms as they represent areas where the material is most vulnerable under applied loads. The analysis also revealed deformation patterns, showing how the material responds to tensile, compressive, and cyclic loading. This understanding helped optimize the geometry and composition to minimize stress concentrations and enhance overall durability.

3. **Thermal Performance**

   Thermal simulations provided valuable insights into the alloy's behavior under varying temperature gradients. The optimized alloy demonstrated better thermal resistance, with reduced thermal expansion and deformation under high-temperature conditions. This ensures reliability in applications involving extreme thermal environments, such as aerospace and automotive engine components.

Figure 7: Thermal Analysis

4. **Multi-Physics Integration**

   One of the key advantages of the approach was the integration of both mechanical and thermal simulations. This ensured that the optimized alloy could perform reliably under multi-physics conditions, where both thermal and mechanical stresses are simultaneously present. This holistic analysis improves confidence in the alloy's performance for demanding applications.

5.2 Limitations

Despite the success of the project, certain limitations were identified that should be addressed in future studies:

1. **Idealized Models and Boundary Conditions**

   The simulations relied on idealized 3D models and simplified boundary conditions. While these provide a good approximation of real-world behaviour, they do not account for the complexities of actual operating environments. Factors such as environmental conditions, microstructural defects, and manufacturing imperfections were not included, potentially affecting the accuracy of the results.

2. **Absence of Long-Term Fatigue and Creep Analysis**
   Long-term performance indicators such as fatigue resistance and creep (the slow deformation of a material under constant stress) were not included in the current scope. These factors are critical for applications involving prolonged exposure to loads and high temperatures, and their exclusion limits the comprehensiveness of the study.
3. **Computational Constraints**
   While efforts were made to ensure mesh accuracy and computational efficiency, some compromises were necessary due to hardware limitations. High-resolution simulations, particularly for complex geometries, may provide even more precise results.

6. Conclusion and Future Work

Conclusion

This project successfully demonstrated the use of Finite Element Analysis (FEA) in optimizing the mechanical and thermal properties of a selected alloy. By systematically varying the alloy composition and analysing its response to mechanical loads and thermal gradients, significant enhancements in performance were achieved. Key outcomes of the study include:

1. **Improved Mechanical Strength**
   The optimized alloy exhibited superior mechanical properties, including higher yield strength and better resistance to deformation under tensile and compressive loads.
2. **Enhanced Thermal Stability**
   The alloy’s resistance to thermal expansion and deformation was significantly improved, ensuring reliability in high-temperature applications.
3. **Stress Concentration Mitigation**
   Through geometry optimization and compositional adjustments, stress concentrations were minimized, reducing the likelihood of failure under extreme conditions.

While the project successfully achieved its objectives, it also highlighted the potential for further improvements, particularly in incorporating real-world complexities and advanced optimization techniques.

Future Scope

To build upon the findings of this study, several areas of future work are proposed:

1. **Experimental Validation**
   Real-world testing of the optimized alloy is essential to validate the simulation results. Physical experiments will help account for factors not included in the simulations, such as manufacturing defects, microstructural variations, and environmental effects. This validation will provide greater confidence in the alloy's performance for industrial applications.
2. **Advanced Optimization Techniques**
   Leveraging emerging technologies such as artificial intelligence (AI) and machine learning can significantly enhance the alloy optimization process. By analyzing large datasets of material compositions and their properties, AI algorithms can predict optimal configurations more efficiently, reducing the need for iterative simulations.
3. **Multi-Physics Analysis**
   Expanding the scope of simulations to include additional physical phenomena such as wear, corrosion, and fluid-structure interactions will further enhance the alloy’s applicability. For example, wear simulations can predict the material's durability under abrasive conditions, while corrosion simulations can evaluate its resistance in harsh chemical environments.
4. **Inclusion of Long-Term Studies**
   Incorporating fatigue analysis and creep studies into the simulation framework will provide a more comprehensive understanding of the

material's long-term behavior. This is especially important for applications involving continuous exposure to stress and elevated temperatures.

5. **Application-Specific Customization**

   Future work can focus on tailoring the alloy's properties for specific applications, such as aerospace, automotive, or heavy machinery. This will involve customizing the composition and geometry to meet the unique requirements of each field

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