Course Project Report

Multiscale Modelling of Materials using Machine Learning

TEAM 3

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1. Component Scale Simulation using FEM

Project Goal: Optimizing Grain Size in Copper Heat Pipes for Enhanced Thermal Efficiency and Stress Management.

Model Setup:
A copper pipe with an inner diameter of 8 mm, outer diameter of 10 mm, and length of 100 mm was created to simulate real-life conditions in heat transfer applications.

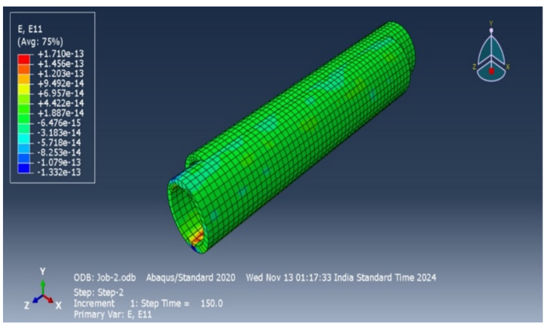
Material Properties:
The material for the heat pipe is copper, characterized by the following mechanical properties:

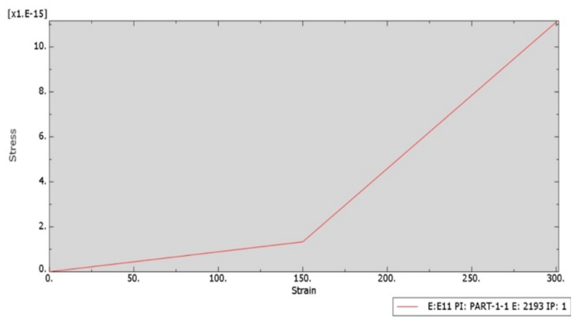
Material Properties:
- Young's Modulus (E): 110GPa – shows material stiffness.
- Poisson's Ratio (ν): 0.33 – indicates lateral expansion when stretched.
- Yield Stress: 285 MPa – the stress limit before permanent deformation.
- Strain hardening exponent – 0.2.

Loading and Boundary Conditions:
A radial load of 200 units of displacement was applied to the inner surface of the pipe, representing forces the pipe might experience during heat transfer. Both ends of the pipe were left free to move, so only the radial response was observed.

Mesh and Element Type:
The model used a 3D mesh with square elements, each side 2 mm long, to capture detailed stress and deformation patterns.

Objective of the Simulation:
The goal is to study **stress, displacement, and strain** in the pipe under load, which helps identify weak areas and improve design for better performance and durability.





2. Importance of Microstructure Details (Grain Size and Dislocation Density)

1. **Need for Microstructural Details in Materials:**

   Microstructural details, like **grain size and dislocation density**, play a critical role in determining a material's performance, especially under thermal and mechanical loads. Smaller grains often increase a material's strength (Hall-Petch effect) by limiting dislocation motion, making it more resistant to stress and deformation. Dislocation density, which refers to the number of dislocations within the grains, also impacts strength and ductility. These microstructural characteristics directly affect **heat transfer efficiency, stress resistance, and the material's overall durability**.

2. **Microstructural Details Simulated in Copper Heat Pipe:**

   In this study, **grain sizes from 5 to 95 microns** were tested across **four different strain rates (10^-2 to 10^-5)**. The results indicated that **stress levels increase as grain size decreases**. This means that copper with smaller grains can withstand higher stress, which is beneficial for structural stability in high-heat and high-stress conditions typical of heat pipes.

3. **Effect on Heat Pipe Efficiency:**

   The findings suggest that **optimizing grain size** in copper can enhance both **stress tolerance** and **heat transfer performance**. Using copper with finer grains in heat pipes could improve their ability to endure mechanical and thermal stresses, potentially increasing the efficiency and lifespan of heat transfer systems.

3. Multiscale Modeling Strategy

Purpose of Multiscale Modelling:
Multiscale modeling helps us understand how small-scale material details, like grain size and orientation, affect the larger structure. By incorporating these microscale properties into our FEM simulation, we get a more accurate view of how the copper heat pipe behaves under stress.

Connecting Microscale to Macroscale:
To link the micro and macro scales, we use microscale data (like grain behavior) to inform the larger FEM model. Here, we employ a **polynomial regression-based model** that adjusts the material properties based on grain size, which is then applied to the macroscale FEM simulation.

Benefits of This Integration:
By including grain-level details in the macroscale model, we can better predict stress distribution and deformation in the copper heat pipe, improving accuracy in simulating how it will perform under real conditions.

4. VPSC Model Setup and Microstructure Integration

VPSC Model Configuration:
To set up the **VPSC (Visco-Plastic Self-Consistent) model**, we used Fortran to run the simulation code. We modified two key files:

- **tension.1:** This file was used to adjust the **strain rate values** for four different levels, which helped simulate the effect of varying loading conditions on the material.
- **copper.sx:** Here, we changed the **grain size** for 19 different values to understand how varying grain sizes impact the material's behavior under different strain rate.

Microstructure Representation:
The microstructure of copper was accounted for by modifying the grain size and strain rate in the VPSC model. This allowed us to simulate how **grain orientation** and **size** influence the material's **plastic deformation** and **stress distribution** under different loading conditions, providing a realistic representation of copper's behavior in the heat pipe simulation.

5. Database Generation as a Function of Strain Rate and MicrostructurePurpose of Multiscale Modelling:

1.**Dataset Creation Process:**
To generate the required dataset, we ran the **VPSC simulation** 76 times using the **vpsc7.exe** file. For each run, we set a **step size of 100** and varied the **strain rate** between **10^-2 and 10^-5** (modified in the **tension.3** file) and the **grain size** from **5 to 95 microns** (modified in the **copper.sx** file). Each simulation provided stress-strain data c orresponding to the specific combination of strain rate and grain size.

2.**Utility for Machine Learning:**
This generated dataset, containing **76 unique combinations** of stress, strain, strain rate, and grain size, serves as the foundation for the **machine learning model**. By analyzing this data, the ML model can learn how **grain size and strain rate** influence the material's behavior, which is crucial for predicting the copper heat pipe's performance under varying conditions.

6. Development of Constitutive Model using ML

1. **Dataset Preparation:**
First, we concatenated the dataset generated from the VPSC simulations, which included stress, strain, strain rate, and grain size. We then split the dataset, using 80% for training and 20% for testing the model.

```
df_merged = pd.concat([locals()[f'df_{i}'] for i in range(1, 77)], axis=0)
[16] ✓ 0.0s

df_merged
[17] ✓ 0.0s
```

	E11	SCAU11	strain_rate	grain_size
0	0.000000	162.830000	0.01000	0.000005
1	0.000667	163.296667	0.01000	0.000005
2	0.001429	163.801429	0.01000	0.000005
3	0.002267	164.366000	0.01000	0.000005
4	0.003161	165.033871	0.01000	0.000005
...	...	...	...	...
96	0.095000	111.948127	0.00001	0.000095
97	0.096000	112.259063	0.00001	0.000095
98	0.097000	112.569532	0.00001	0.000095
99	0.098000	112.874766	0.00001	0.000095
100	0.099000	113.177383	0.00001	0.000095

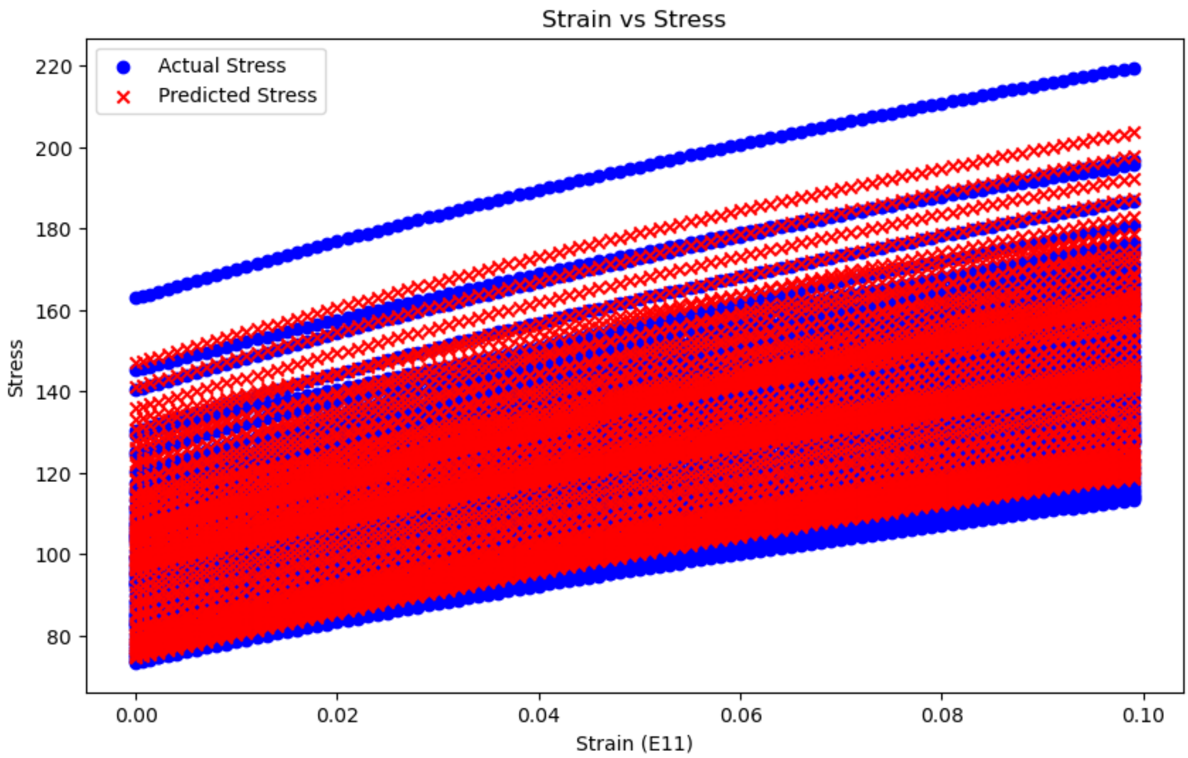
7676 rows × 4 columns

2. **Polynomial Regression:**
Using the training dataset, we applied polynomial regression (degree 2) to model stress as a function of strain, strain rate, and grain size. These variables were treated as input variables, while stress was the output variable. The model was trained to learn the relationship between these inputs and the resulting stress.

3. **Equation Development:**
After training, we plotted the stress-strain relationship and derived the coefficients and intercepts. The final constitutive equation based on the polynomial regression is as follows:

Stress (SCAU11) = 115.87000 + (581.17094) * E11 + (24694.12860) * strain_rate + (1168663.06000) * grain_size + (-1368.07412) * E11^2 + (12543.13140) * E11 * strain_rate + (-29095.13080) * E11 * grain_size + (-2102507.11000) * strain_rate^2 + (-9820971.89000) * strain_rate * grain_size + (8222685370.00000) * grain_size^2

This equation represents the relationship between the stress, strain, strain rate, and grain size in the copper heat pipe and can be used for further simulations and predictions of material behavior under different loading conditions.



Machine Learning Evaluation
Mean Squared Error: 31.44034706052648
R-squared: 0.9485657844102036

7. UMAT Code and ML-Derived Constitutive Law Integration

The UMAT code in FEM allows us to define custom material behavior, which is essential for incorporating the ML-derived constitutive law.

1.Stress Flow Equation Integration:
In the UMAT code, we integrated the stress equation derived from the machine learning model by defining it as the sf variable. To incorporate the material's plastic deformation behavior, we differentiated the stress equation with respect to eqplas (plastic strain). Additionally, we updated both the stress (sf) and strain tensor (et) by adding dequal, which represents the accumulated plastic strain. This integration allows the FEM model to dynamically adjust the material's stress-strain behavior based on the microstructure, as informed by the ML-derived model.

2.Dynamic Stress-Strain Adjustment:
The ML-derived equation is used in the UMAT subroutine for Isotropic Strain Hardening. At each step of the FEM simulation, this equation adjusts the stress-strain relationship based on the local grain size and strain rate. This dynamic adjustment is crucial because it accounts for microstructure heterogeneities, unlike simpler models that assume uniform material response.

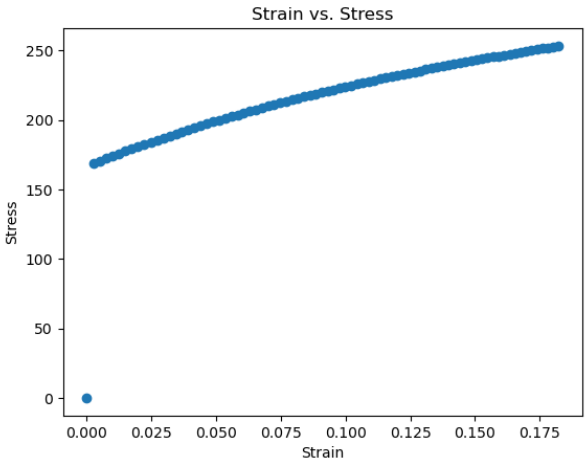
This integration enhances the accuracy of the FEM simulation by providing a more detailed and localized representation of the material's behavior under stress.

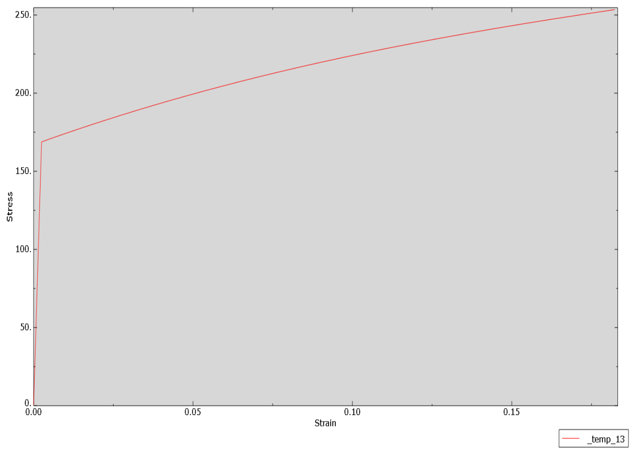
8. Validation of FE-UMAT Against VPSC Simulation Results

Validation Method:
To check the accuracy of the ML-based UMAT model, we ran single-element FE simulations. We compared the stress-strain results from the UMAT code with the VPSC model results, using a grain size of 65 microns and a strain rate of 10^{-2}. This helped ensure that the UMAT model behaves like the VPSC model under the same conditions.

Why Validation is Important:
This step is important to make sure the UMAT model, using the ML-derived equation, can reliably predict how the material will react based on changes in grain size and strain rate.

Graph Comparison:
The graph below shows the stress-strain results from both UMAT and VPSC. The close match between them confirms that the UMAT model is accurate.





VPSC Plot

ML Enhanced UMAT Plot

9. FEM Model Geometry, Mesh, and Microstructure Description

The FEM model was set up with a solid copper pipe with diameter 10mm and length 100mm, where one end was fixed and a tensile load of 200 units was applied to the other, simulating the forces during heat transfer. The mesh used square elements with an edge length of 2, refined to capture localized effects influenced by the microstructure.

In the VPSC model, uniform material properties were applied, while the ML-based model incorporated grain size distribution through the UMAT subroutine. This approach allowed for a more realistic simulation, accounting for the material's microstructural heterogeneity.

10. Results and Discussion: Impact of Heterogeneous Microstructure

We compared FEM simulations of copper heat pipes with and without microstructure (grain size).

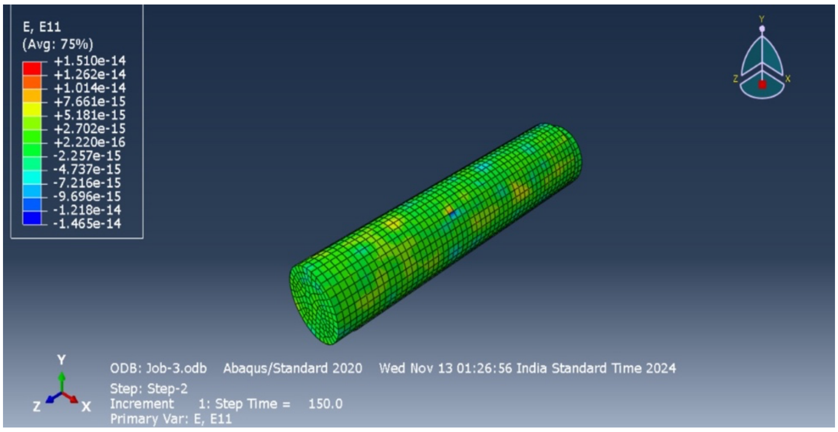
1) **With Microstructure:** The ML-based model, accounting for grain size, showed significant stress variations and strain localization. As grain size decreased, stress increased, highlighting the importance of microstructure for accurate deformation predictions.

2) **Without Microstructure:** The VPSC model, lacking microstructure details, showed a more uniform material response.

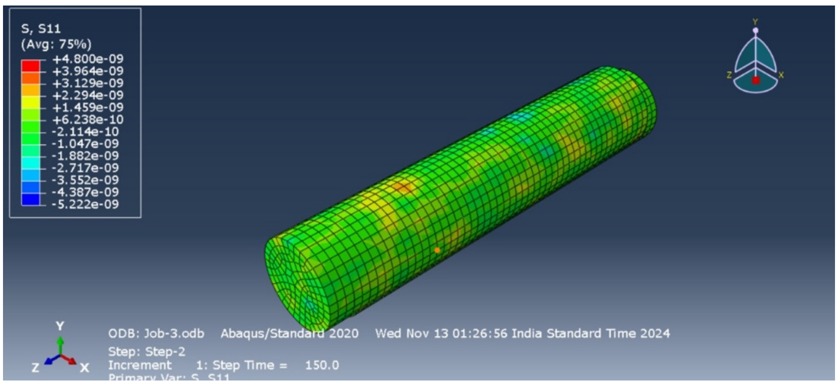
This comparison demonstrates that grain size significantly affects material behavior, providing deeper insights into how microstructure influences deformation and performance.

Results and Plots:

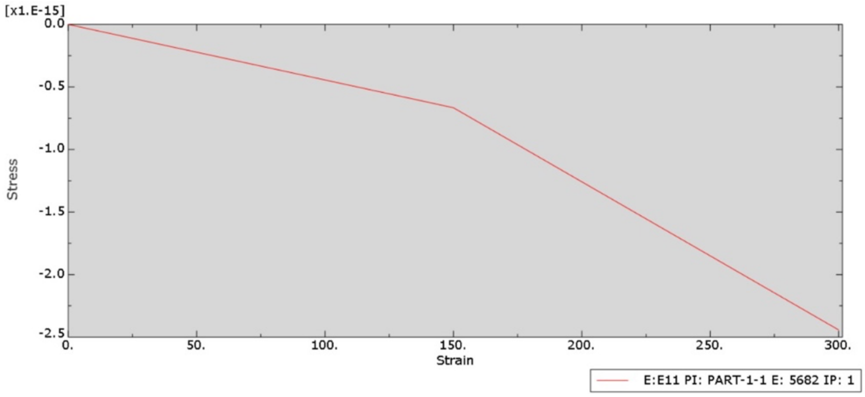
1) Stress vs Strain Analysis when grain size is introduced.



Strain Distribution

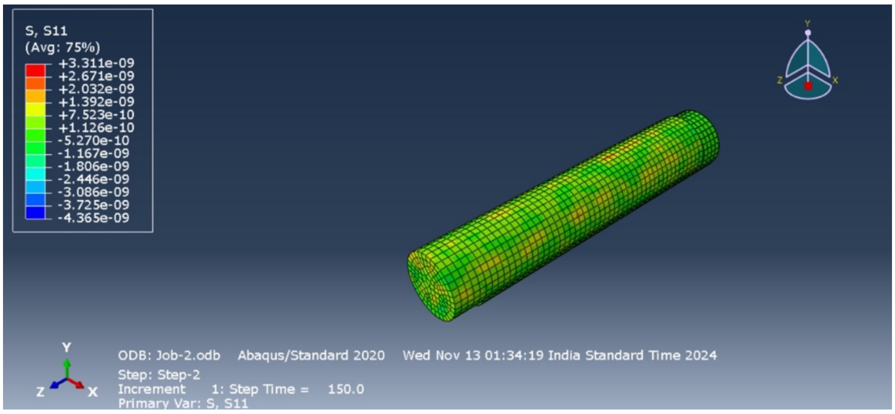


Stress Distribution

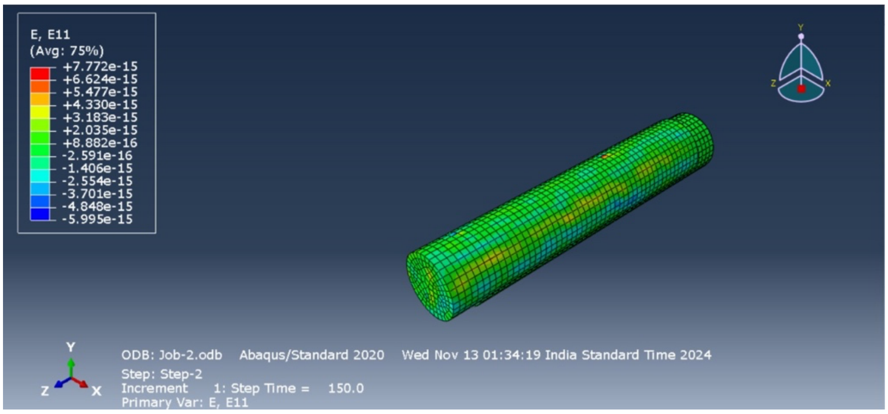


Strain vs Stress with microstructure included

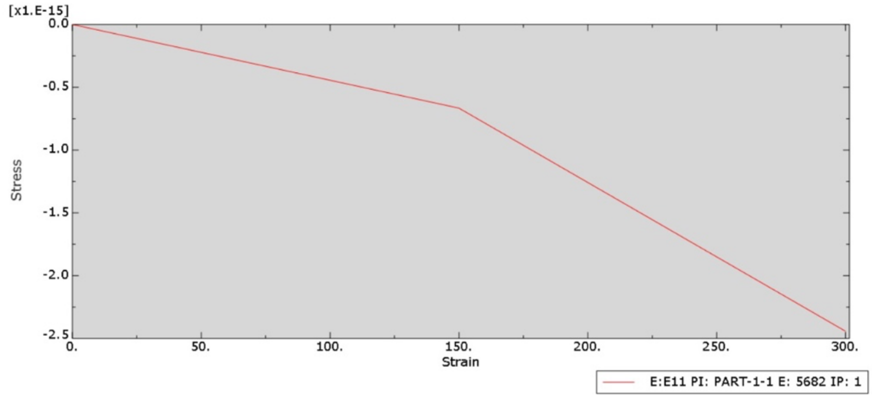
2) Stress vs Strain when the grain size in not introduced



Strain Distribution



Stress Distribution



Strain vs Stress with microstructure not included.

Conclusion:

The project successfully integrated microstructural details like grain size into the FEM simulation of a copper heat pipe. By varying grain sizes and strain rates, it was found that smaller grain sizes enhance the material's strength. The optimal grain size for copper heat pipes is around 10-20 microns, balancing mechanical strength and thermal conductivity for better performance in heat transfer and deformation behavior. This integration of microstructure in simulations provides valuable insights into material behavior and improves the accuracy of heat pipe model.