# Multiscale Modelling of Materials using Machine Learning

*A Project Report*

*submitted by*


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*in partial fulfilment of requirements for the completion of the project work of Multiscale Modelling of Materials using Machine Learning.*


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# 1 Description of the component scale simulation using FEM

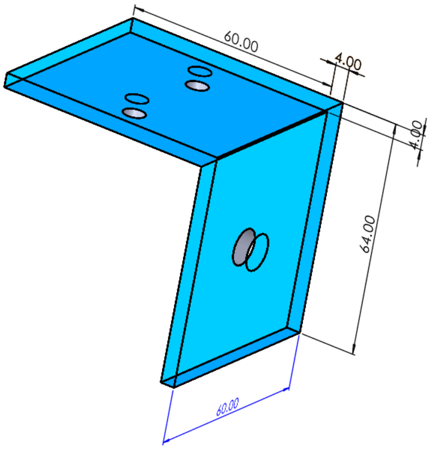



Figure-1 : CAD Dimensions 1

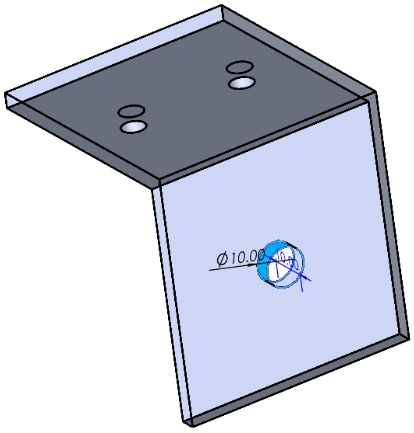



Figure-2 : CAD Dimensions 2

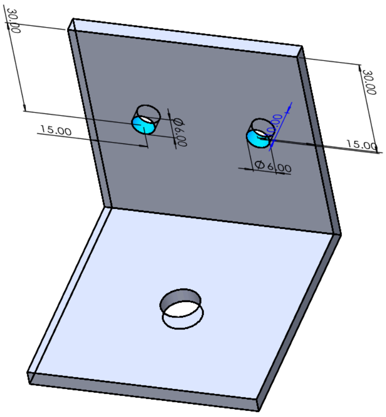



Figure-3 : CAD Dimensions 3

An L-Bracket has been modelled in Solidworks (CAD), all dimensions are in mm. For performing FE simulations, ABAQUS 2020 software was decided to use. Bringing in the custom material properties (grain size) using UMAT subroutine into FE simulation.

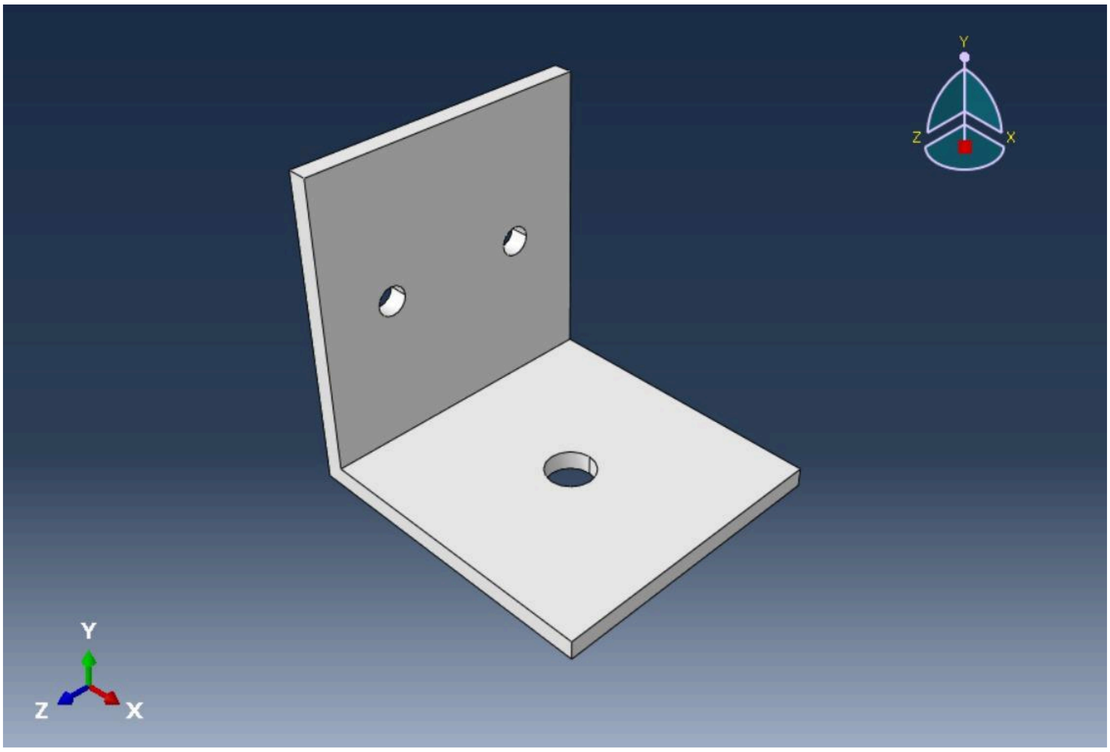



Figure-4 : Part Geometry

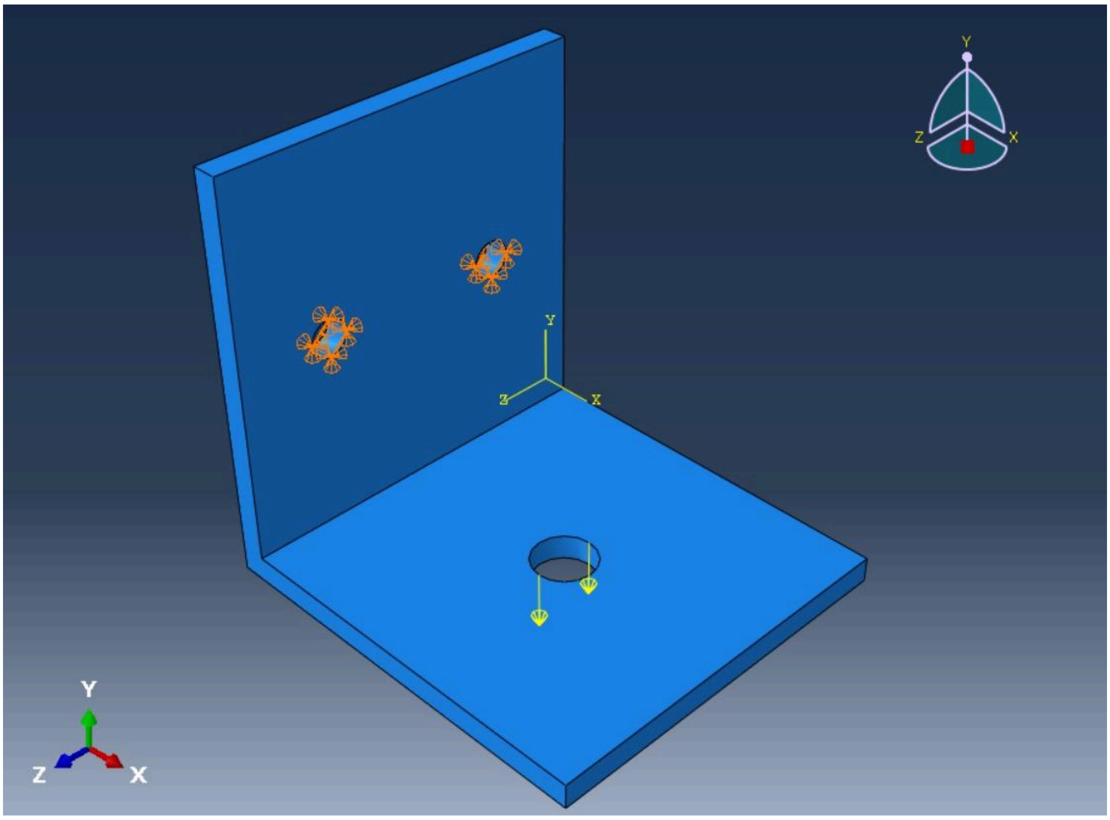



Figure-5 : Boundary Conditions and loading.

Two holes whose constraints are highlighted in orange have been constrained for x, y and z displacements.

Load highlighted in yellow colour loaded 2000N in negative y direction. (Figure-5)

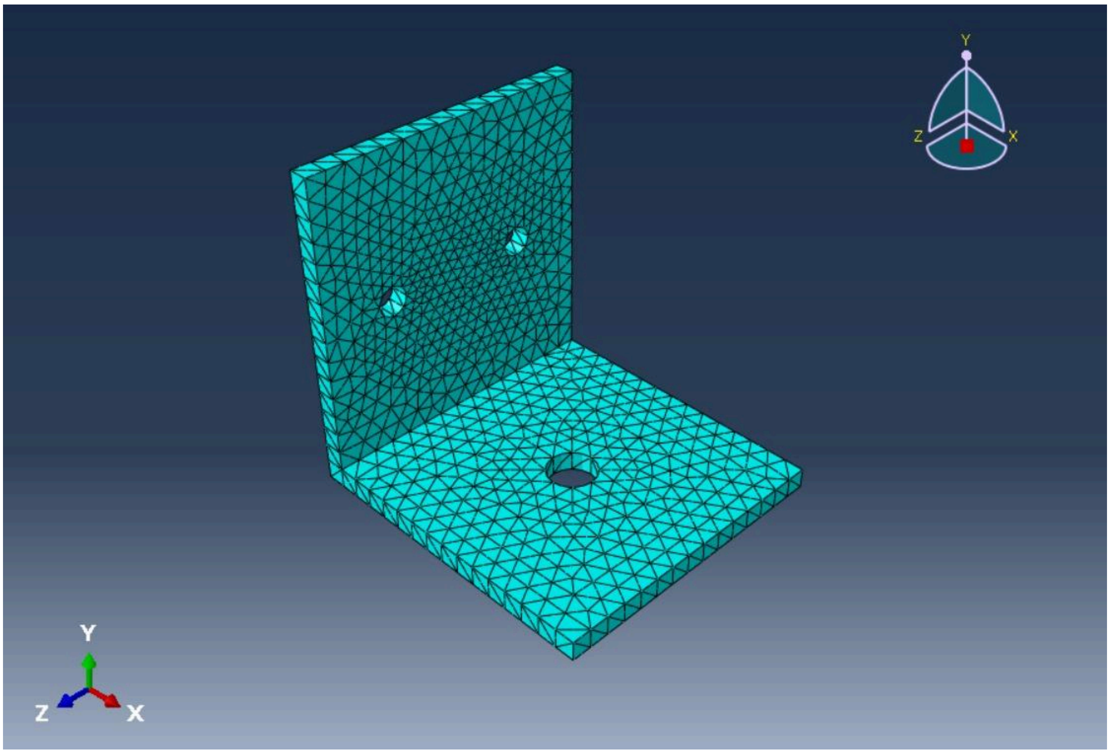



Figure-6 : Meshed geometry

It was difficult to mesh the geometry using hex elements since it was difficult for the algorithm to mesh around the holes, the tetrahedral element was chosen with 4mm size.

User material in ABAQUS takes 4 inputs primarily, young's modulus, poisson ratio, strain rate and grain size.

## 2 Need for microstructure details and its effect

If we bring in the properties of material grain size, we can be much more efficient in the usage of material, by getting into plastic deformations. If plastic deformations need to be understood, it starts from understanding the behavior from micro level, then till macro level going through multiple length scales.

Plastic deformation occurs due to the dislocations and slips in the lattice. Also the grain boundaries are a typical point for initiation of cracks and it also moves when plastically deformed. So, in order to bring all those characteristics from the micrograin level to predict the plastic stress and strain characteristics in macroscale applications, we need to bring in microstructure details and its effect, aiding in efficient usage of material.

## 3 Concept of multiscale modelling

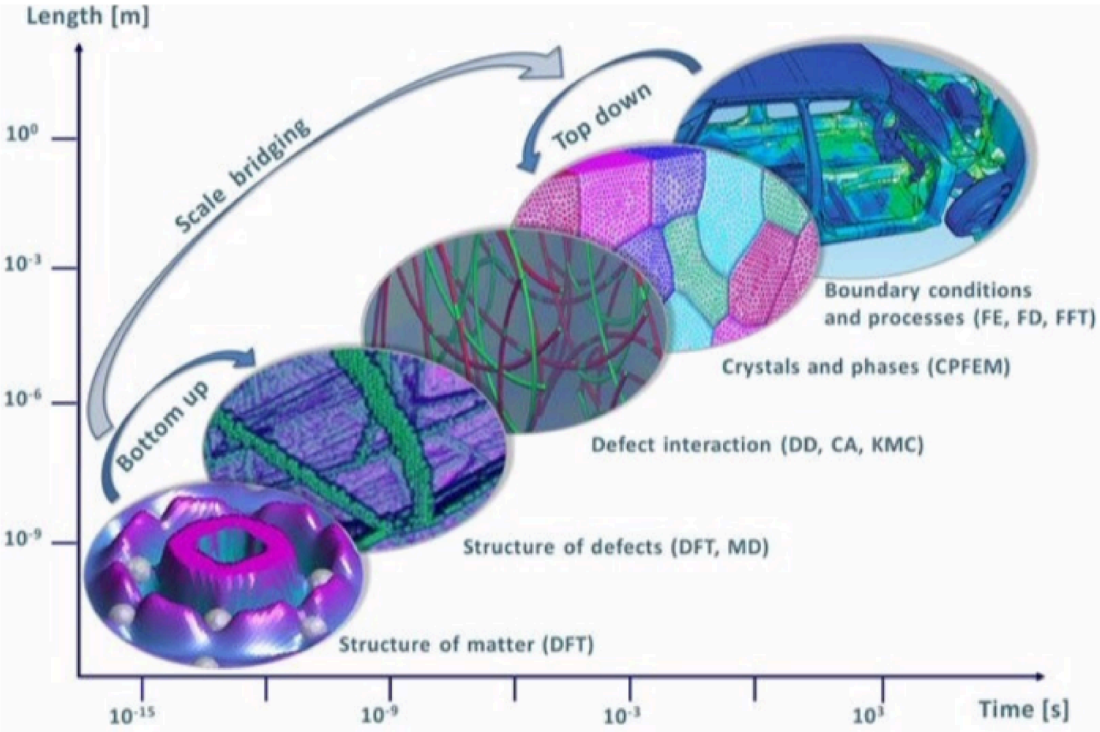



Figure-7 : Multiscale Modelling

The VPSC (Viscoplastic self consistent) model was used to predict the flow stress as a function of plastic strain for different strain rates and grain sizes. Strain rates were between $10^{-2}\,s^{-1}$ and $10^{-7}\,s^{-1}$ for the process to be in quasi static regime. VPSC model accounts for slip planes in a single crystal and gives out stress and strain data for the given grain size and strain rate. We have used the VPSC model to get the stress-strain data for 4 different strain rates and 19 different grain sizes each.

Now, we have a data set with 3876 data points, from this we can predict the flow stress at a given strain, strain rate and grain size by training the data with a machine learning model. The machine learning model will provide us with an equation which relates stress (dependent variable) with strain, strain rate and grain size (independent variables). This equation is provided in the UMAT subroutine file which is linked to FE simulation.

The FE simulation is configured so as to take Young's modulus, poisson ratio, grain size and strain rate as input for the UMAT file. This FE simulation can be done for multiple strain rates and grain sizes to find out the optimal grain size for a particular loading and geometry. This concept of multiscale modelling can be used to prepare a material of the characteristics prescribed by the VPSC model and be used in the given application.

## 4 VPSC model setup and incorporation of microstructure

- VPSC model takes input with aluminium.sx and tension.1, which provides the input data about the microstructure and loading.
  - aluminium.sx has unit cell axes and angles, elastic stiffness, thermal expansion coefficients and grain size.
  - tension.1 contains the number of steps, amount of increment per step and udot matrix which is the strain rate matrix.
- VPSC model is implemented in fortran language so it is required to compile the code and run the executable file.
- The VPSC model then provides us with von mises stress, von mises strain, stress tensor and strain tensor as per axis defined on the VPSC model.
- This was further cleaned and von mises stress and von mises strain were only extracted.

## 5 Database generation as a function of strain rate and microstructure

- The VPSC code was used to populate the database with stress and strain.
- Grain size and strain rate were varied to generate the database.
- Grain size was chosen from 10 to 100 micron with steps of 5 micron amassing to 19 different grain sizes.
- Four strain rate values were chosen ranging from $10^{-2}\, s^{-1}$ to $10^{-5}\, s^{-1}$ .
- A total of 76 (19*4) files with stress-strain output were generated. There were 3876 data points.

## 6 Development of constitutive model using ML

- The machine learning model is developed by using polynomial regression on the dataset.
- Dataset includes the following features:
  - Independent Variables (Inputs): Strain, Strain_rate, and Grain_size.
  - Dependent Variable (Output): Stress
- Applied polynomial feature transformation to capture relationships between the input variables and stress. The polynomial features allow the model to fit complex interactions.
  - poly = PolynomialFeatures(degree=3)
  - X_train_poly = poly.fit_transform(X_train)
  - X_test_poly = poly.transform(X_test)
- Used Polynomial Regression, applied to transformed polynomial features.
  - model = LinearRegression()
  - model.fit(X_train_poly, y_train)
- calculated the R-squared score to assess the model's performance:
  - R^2 Score on Training Data: 0.9998
  - R^2 Score on Testing Data: 0.9997

- Visualization:
  - Stress-Strain Graph: Comparing the actual and predicted stress values to assess model performance.
  - Polynomial Fit Curve: Illustrating how the polynomial model fits the stress-strain relationship, particularly for varying strain values.

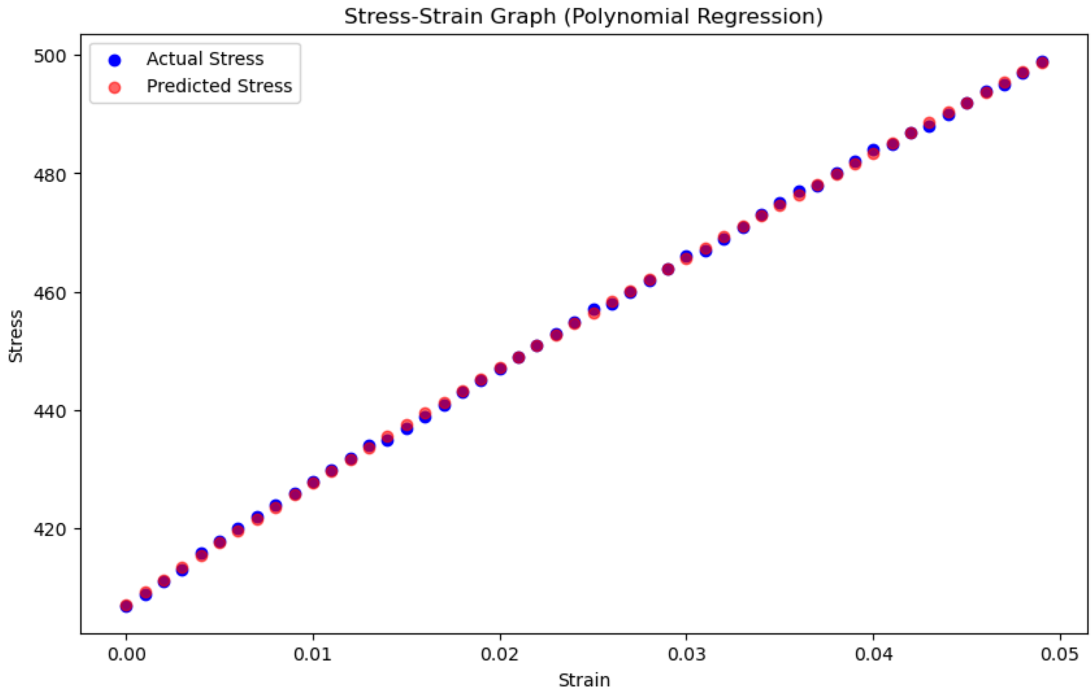



Figure-8 : Tested data plot

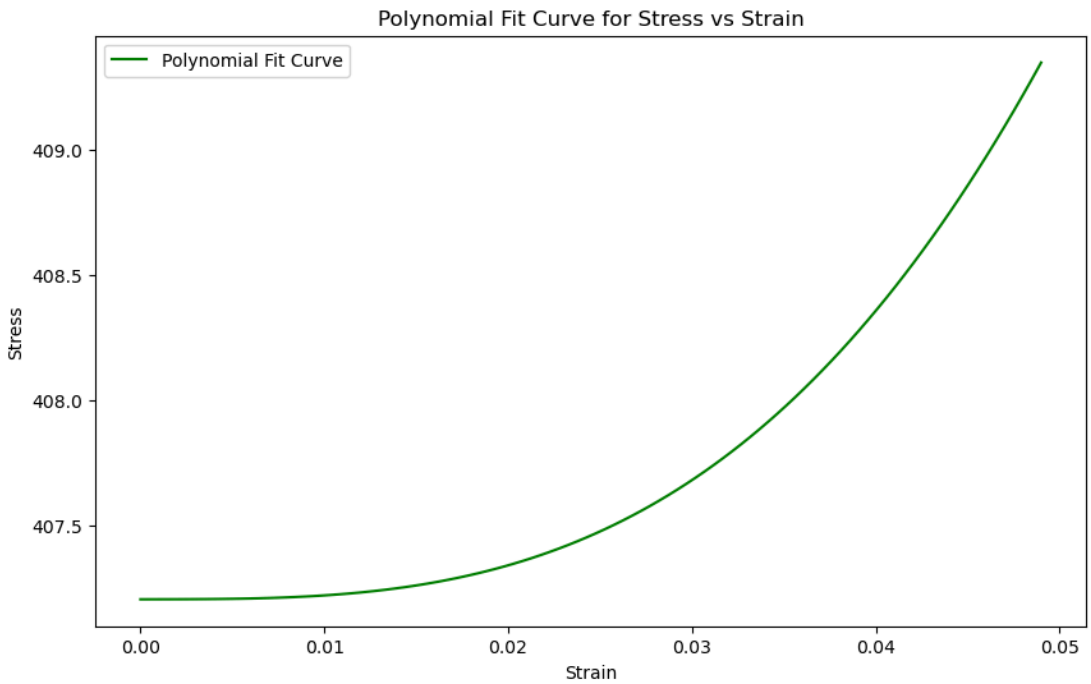



Figure-9 : Polynomial fit curve

# 7 The UMAT code and how it incorporates the ML derived constitutive law

- ➢ The UMAT code takes in the following as input: Young's Modulus, Poisson's ratio, Grain size and Strain rate.
- ➢ It then calculates the Lame's parameters and constructs the elastic jacobian matrix (relates stress and strain).
- ➢ It then calculates the updated stress tensor from the strain increment using elastic jacobian, and Von Mises stress is calculated.
- ➢ Now flow stress is calculated as per plastic strain from the previous increment using ML derived constitutive law.
- ➢ The code then determines if there is active yielding by comparing the Von Mises Stress based on elastic jacobian and flow stress above.
- ➢ if true
    - ○ the flow direction is calculated
    - ○ zero equivalent plastic strain increment is assumed initially
    - ○ Newton-Raphson iteration is performed to update equivalent plastic strain increment
    - ○ The stresses, elastic strain and plastic strains are updated.
    - ○ The jacobian matrix for plasticity is formulated.
- ➢ Elastic strain and plastic strain are stored in state variables to be called in the next iteration.

# 8 Validation of FE-UMAT code against VPSC simulations results using single element FE calculations

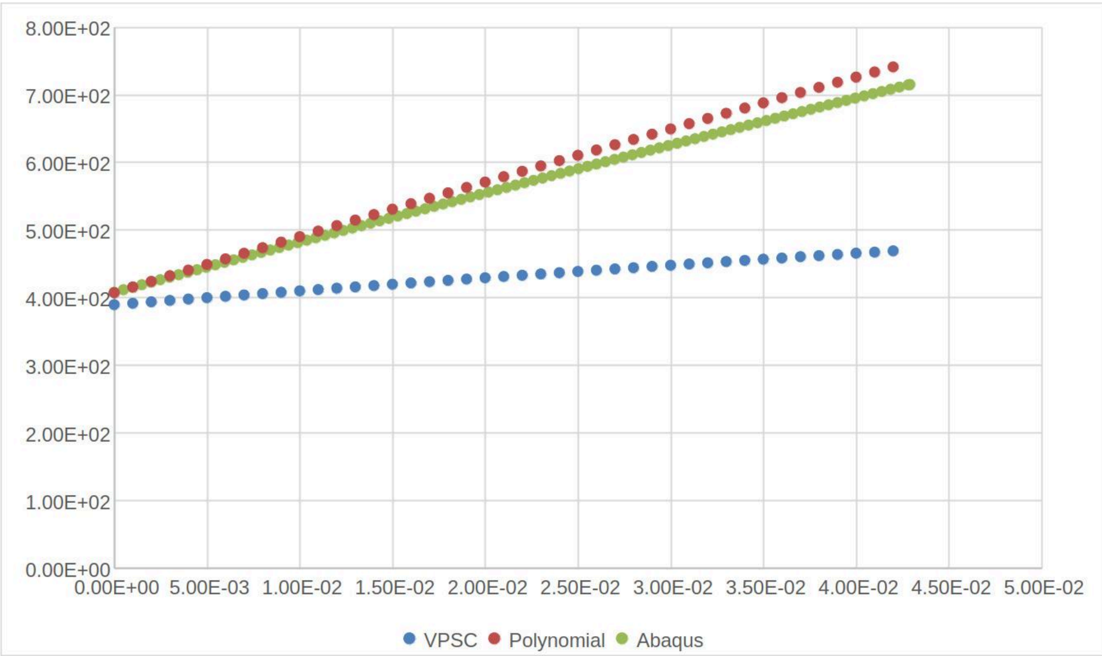



Figure - 10 : Validation Plot

The VPSC model data and when plotted with values predicted by ML model for a given strain rate(0.01) and grain size(20 micrometers) were not agreeing as shown in the above figure in spite of having r^2 value on testing data as 0.9997.

After trying some other strain rates, grain sizes and degree of polynomial for validating the results were not as expected.

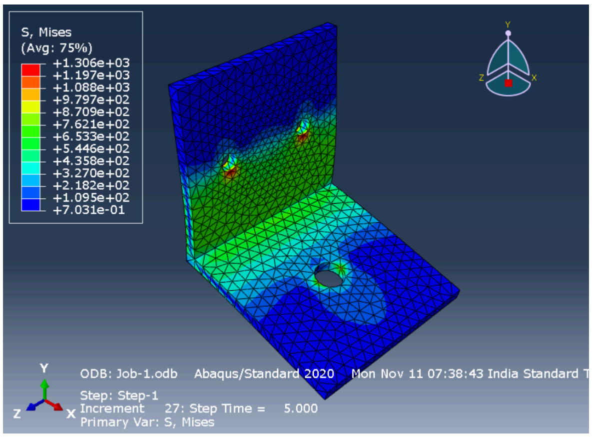
When tried with degree 2 and degree 4, the predictions were far more deviant when its values were compared with VPSC simulated actual values.

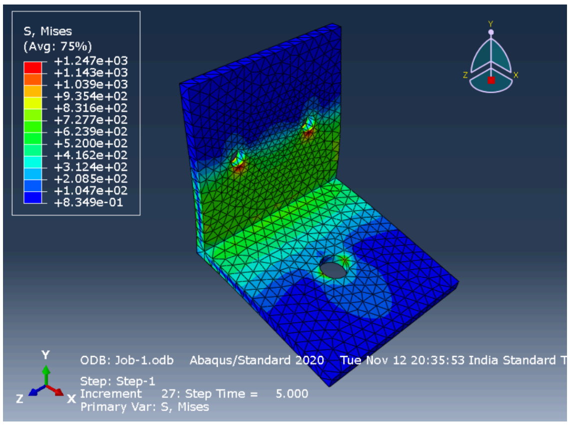
Since we were not able to reason the same, we used the third degree polynomial predicted by the ML model as the constitutive model knowing it was wrong.

# 9 FEM model geometry generation, mesh details and explicit description of the microstructure

- The FEM model was meshed using the tetrahedral element with a mesh size of 4mm.
- Tetrahedral was chosen as it was easier to fit it around the holes over the hex element.
- There were 6969 elements and 12350 nodes
- The mesh size was taken to be 4mm as the thickness of the aluminium sheet (4mm) so that the meshing is done in a single layer.
- The material chosen (Aluminium) has FCC crystal structure.
- The slip system for the chosen material is <111>{110}
    - where <111> is the slip direction and,
    - {110} is the slip plane

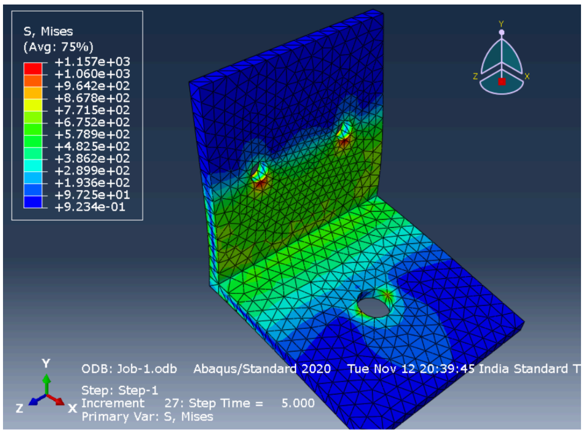
# 10 FEM simulation results and effect of heterogeneous microstructure on the deformation behaviour of materials

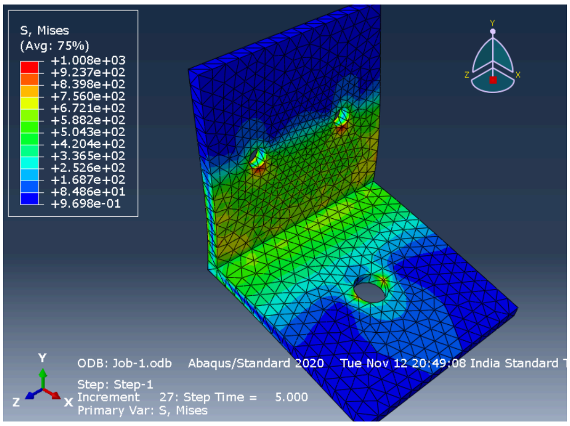



Grain Size -100

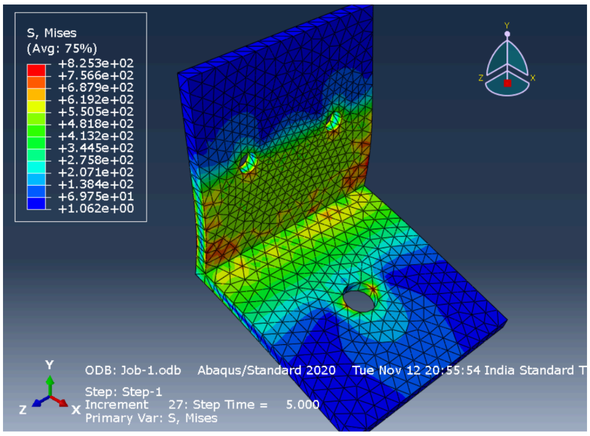
Grain Size - 80

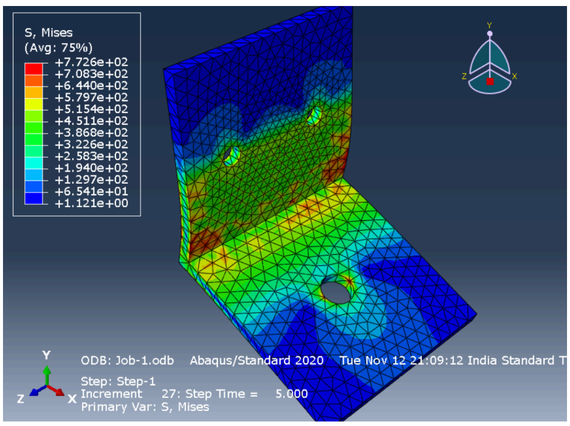



Grain Size - 60

Grain Size - 40




Grain Size - 20

Grain Size - 10

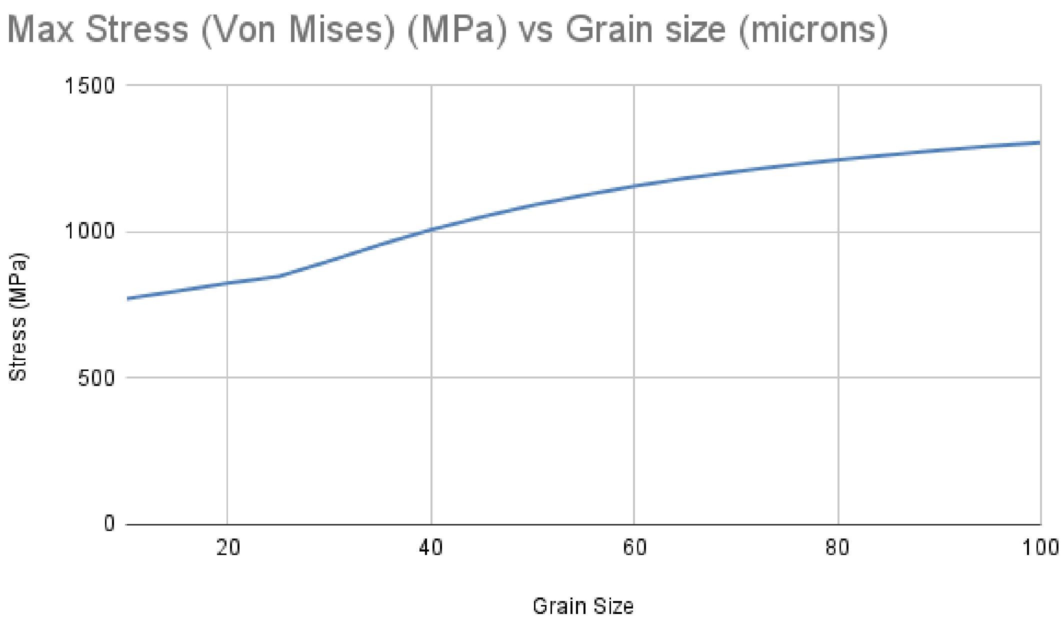



Figure - 11 : Von Mises stress vs Grain Size Plot

From the last plot it is clear that the max von mises stress increases as a function of grain size.

From the FEM plots it is very clear that the stress distribution varies with the grain size.