



**2023 ENGINEERING INSTITUTION OF ZAMBIA  
SYMPOSIUM**

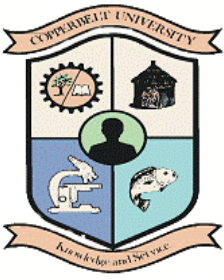
**Trends in materials science based computational models  
for fatigue behaviour of high temperature alloys**

**PRESENTER** : RJ Kashinga; **AW Zulu**; F Banda

**DATE** : **Friday 19<sup>th</sup> April 2024**

**Avani Victoria Falls Resort,  
Livingstone, Zambia**

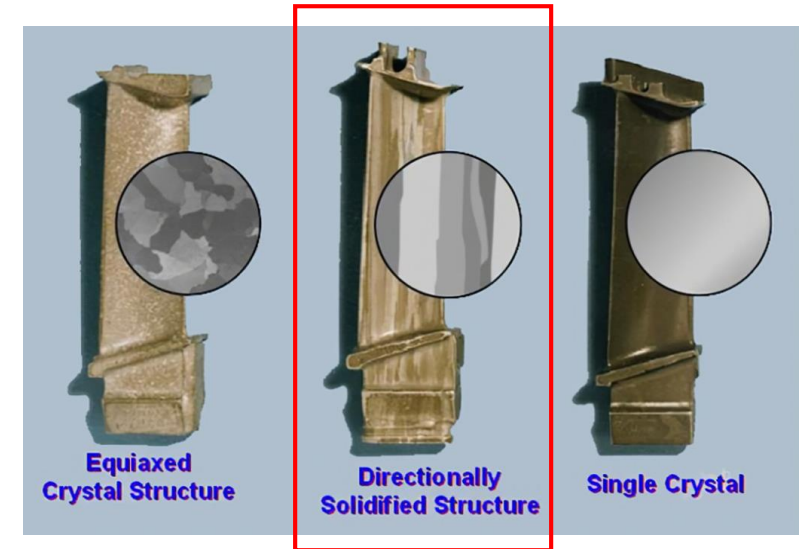
# Introduction



Innovative Engineering curricula to suit existing and future demands and problems

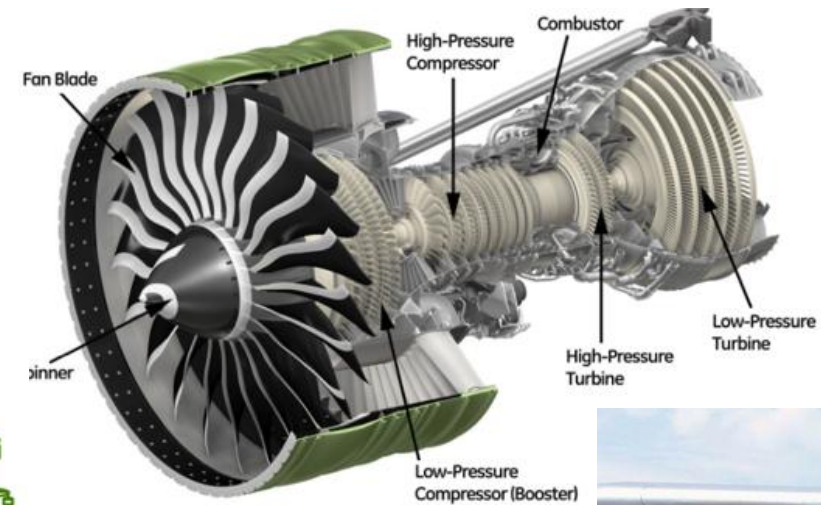
- What are the problems that need solutions from engineers, in today's world??
- What does it take to train an engineer who can solve problems in today's world??
- Is the training being provided in the nation sufficient for engineers??
- What are the challenges?
- How can we improve??
- Training in computational mechanics requires improvement

➤ We look at analysis of failure in a directionally solidified nickel-based superalloy

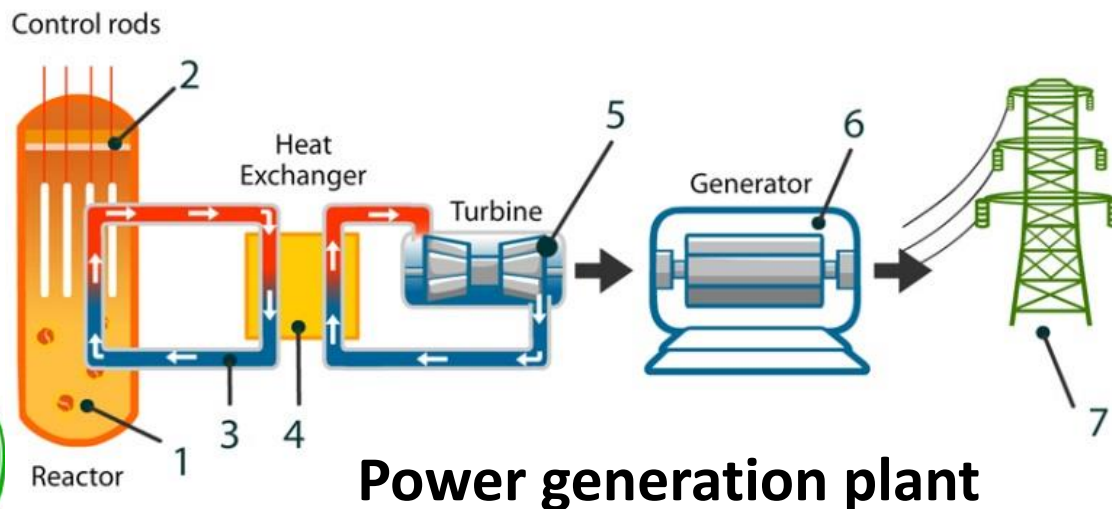


# Introduction

- Ni-based superalloys are materials with unique properties – high temperatures
- Widely used as turbine-engine materials.
- Turbines are widely applied in
  - Power generation
  - Jet engines



Jet engine

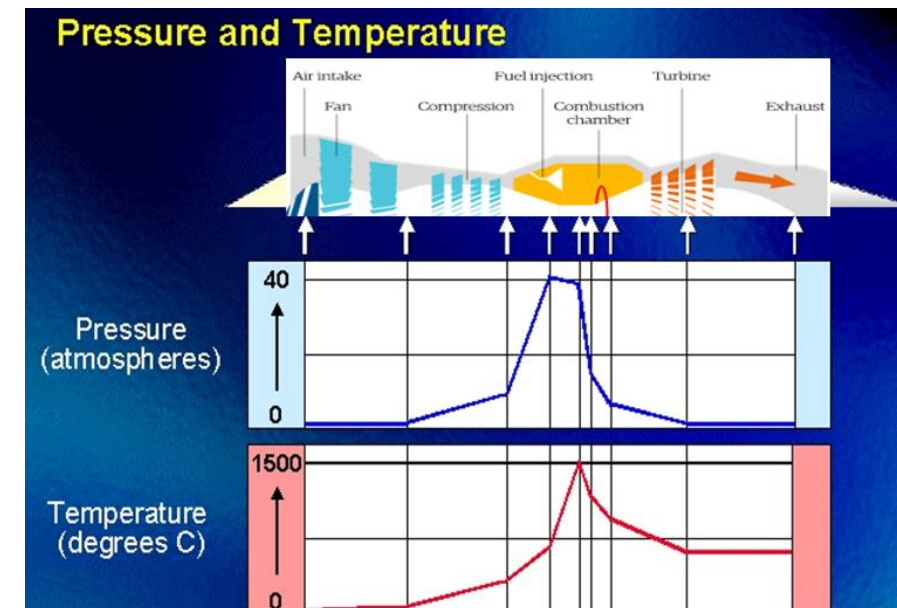
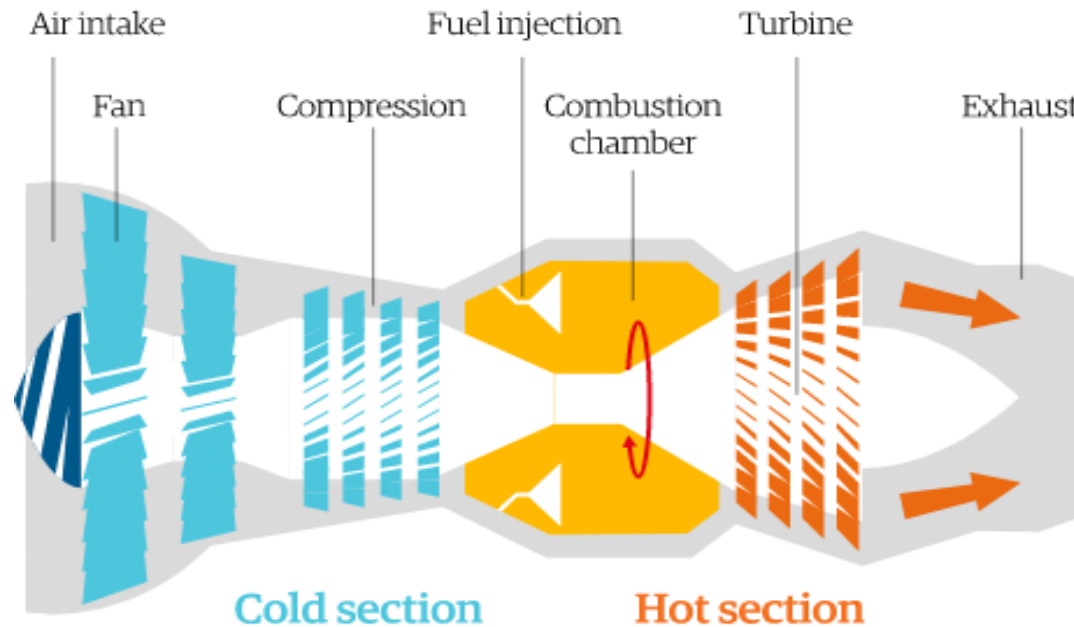


Power generation plant



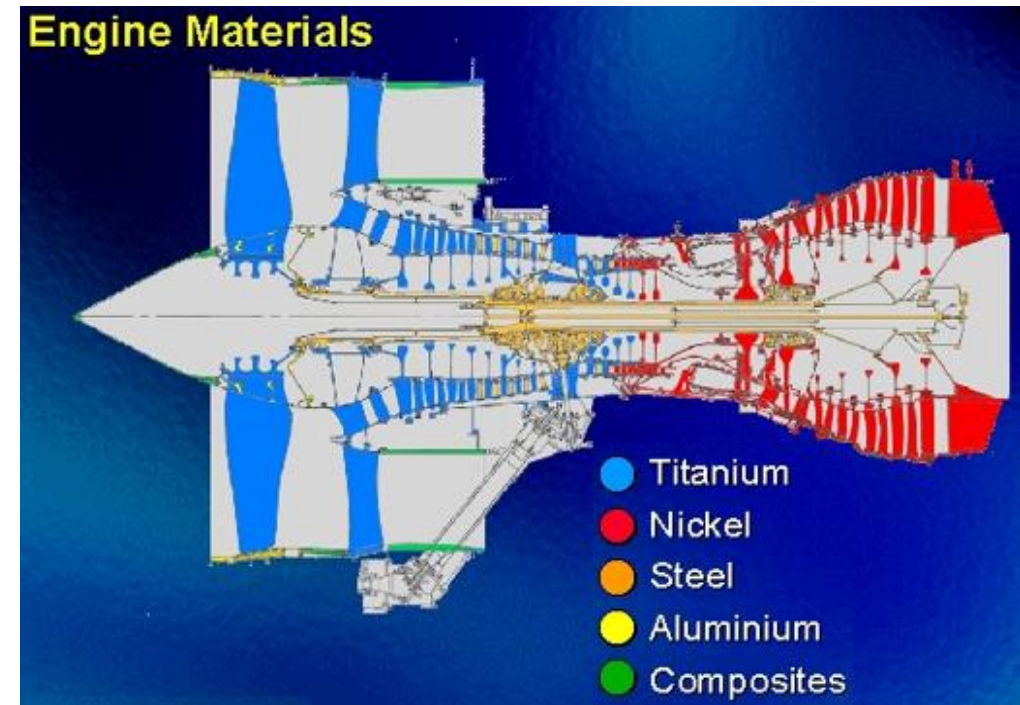
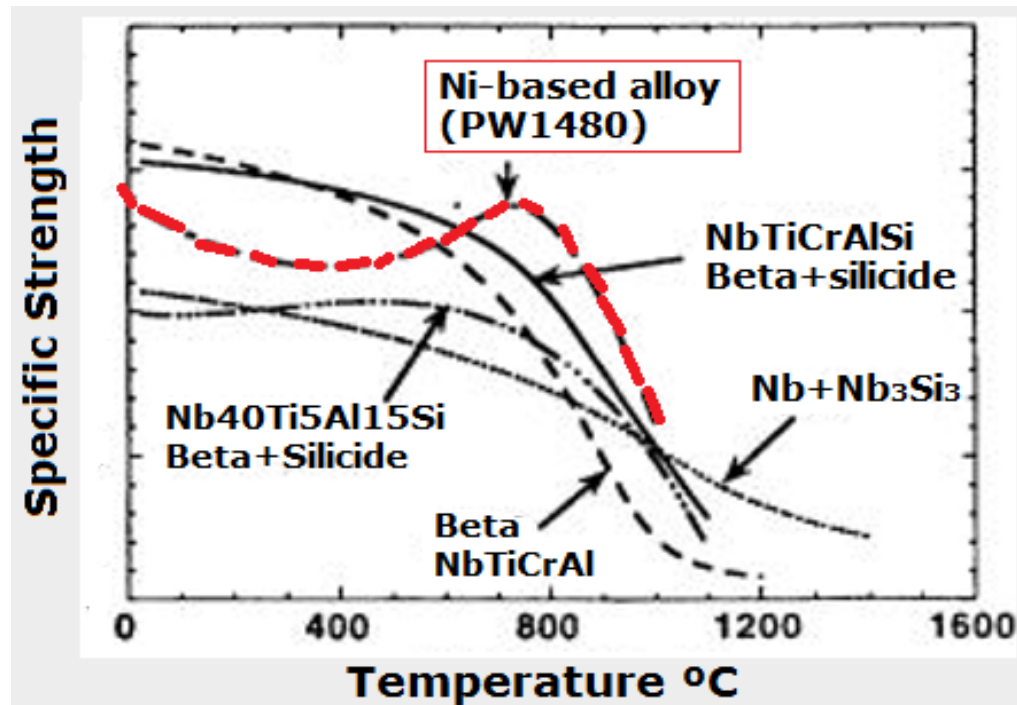
# Introduction

- **Current requirements:- fuel economy, low CO<sub>2</sub>/NO<sub>x</sub> and low noise**
- **Essentials include high:-**
  - ❖ **Compressor exit pressures**
  - ❖ **Turbine temperatures**
- **Materials design is a big challenge.**

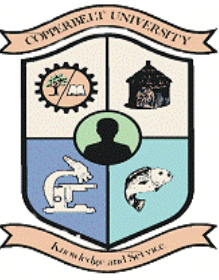


# Introduction

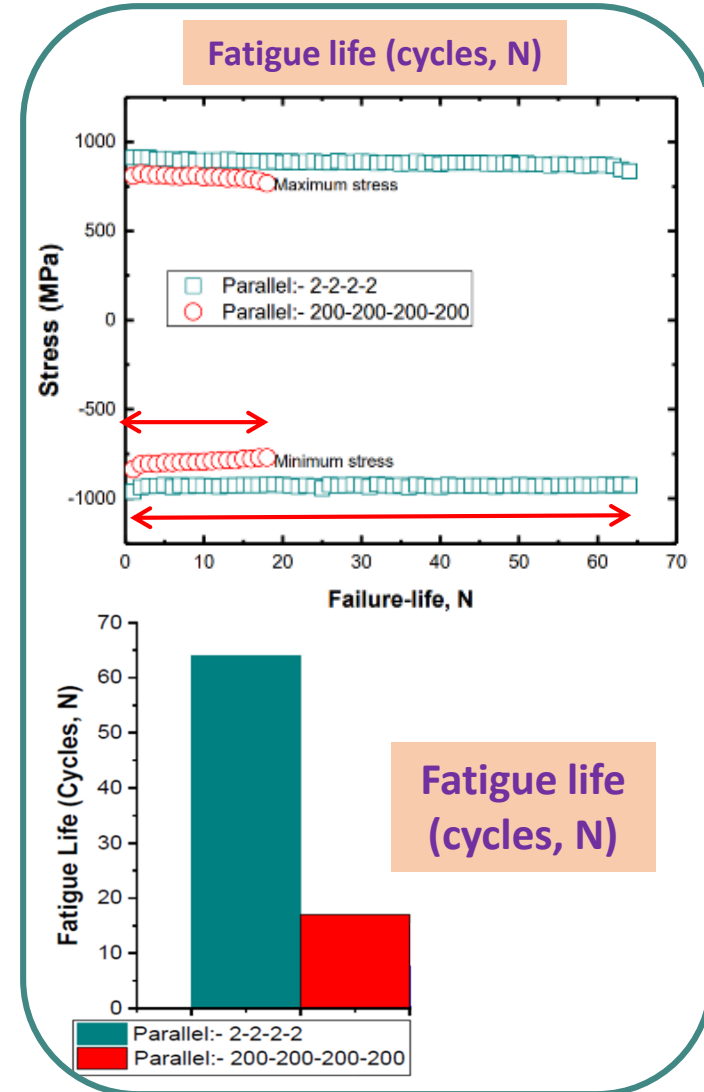
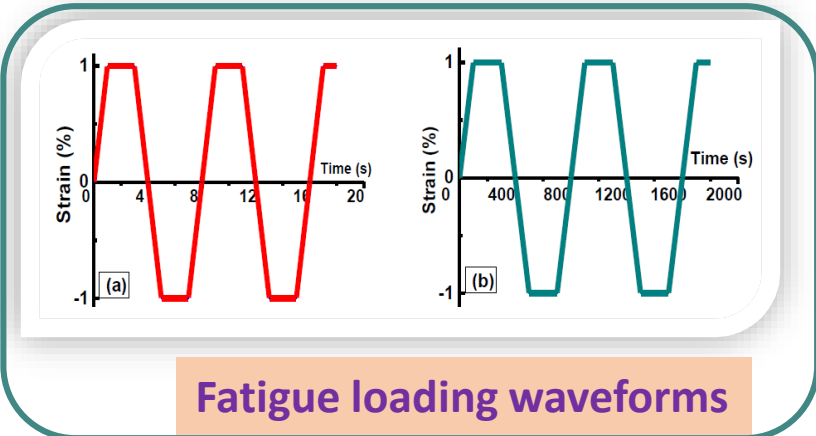
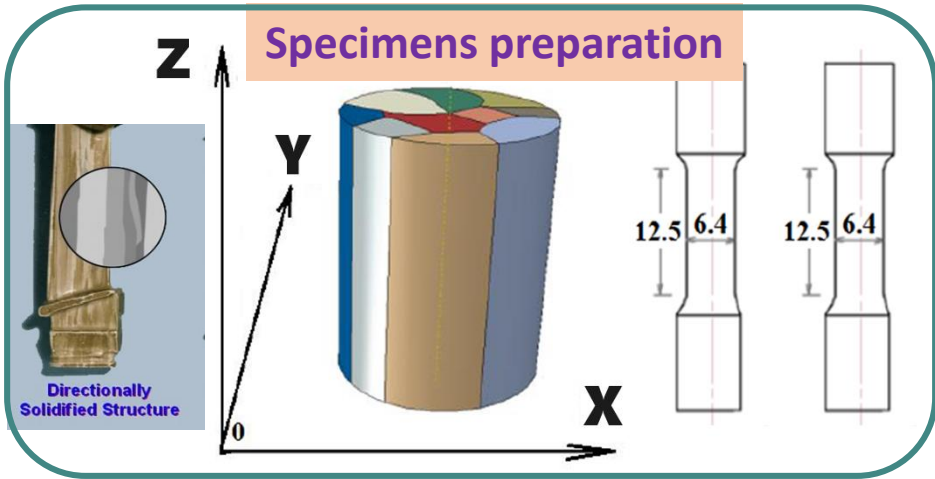
- Steels – historically
- Superalloys – Co-, Ni- and Fe-Ni-based
- Ni-based - extensively applied in hot sections



# Strain-controlled fatigue tests

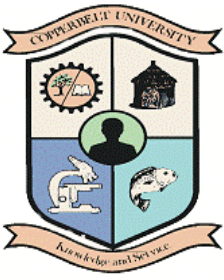


- Two specimens machined from the same sample
- Subjected to fatigue loading, at high temperature
- Results show different number of cycles to failure in the specimens, WHY???
- Investigation, using computational mechanics



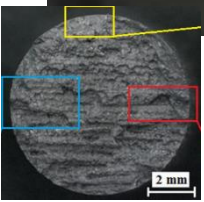
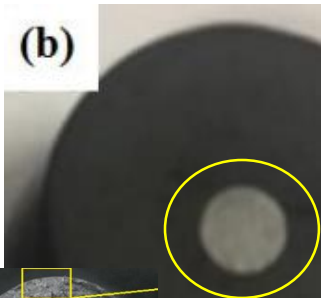
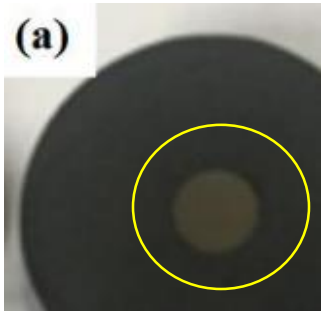


# FE model generation - ABAQUS



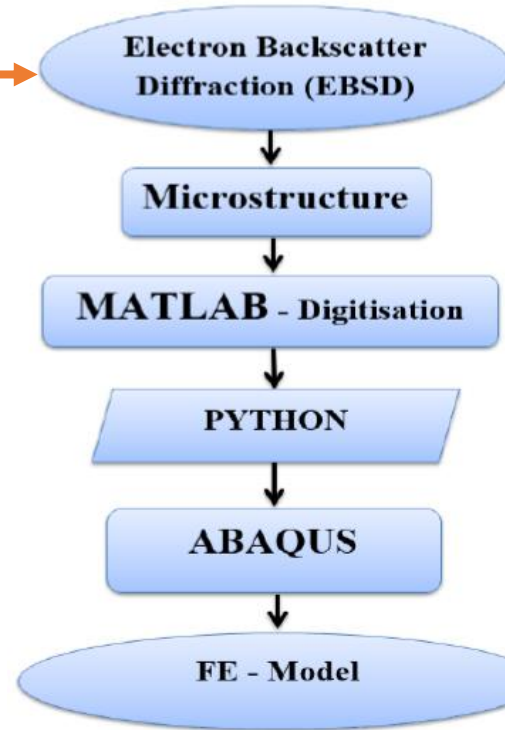
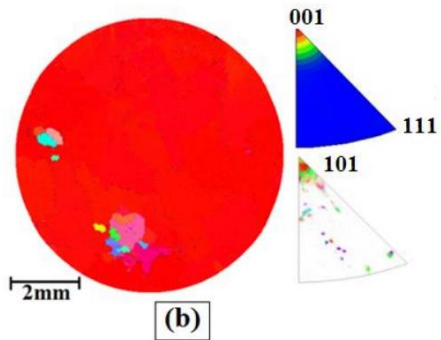
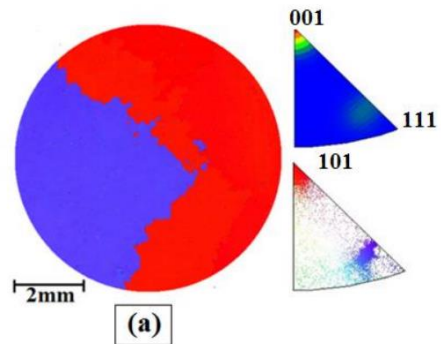
- Two FE models were generated based on the methodology in the flow chart
- Due to curved geometries, mesh was tetrahedral elements
- These are C3D10 with full integration
- Non-uniform mesh size – due to variable grain size

Failed fatigue samples

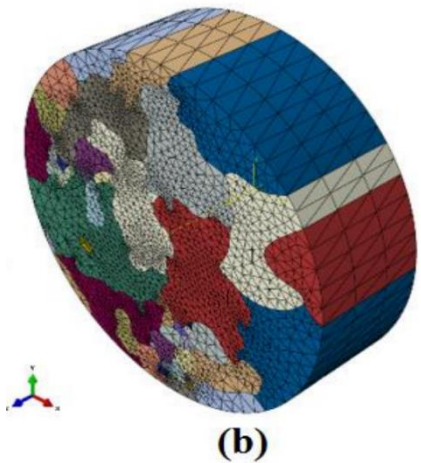
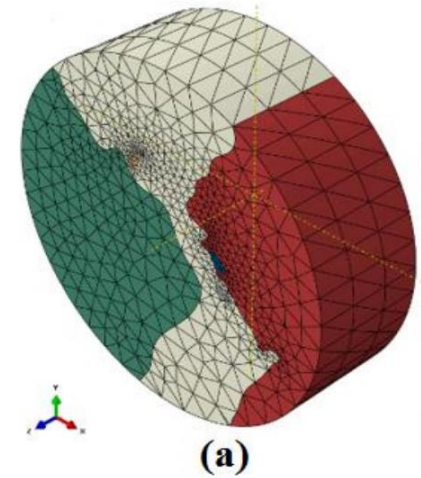


EBSD

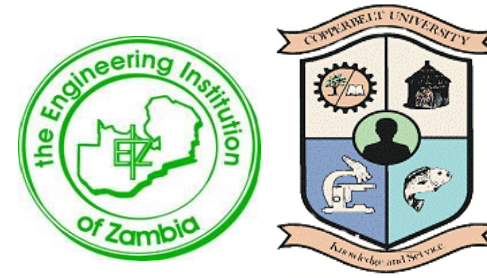
Microstructure from EBSD



FE models



# FE modelling - ABAQUS



- ABAQUS simulations with mechanical deformations – Crystal plasticity model
- Loading & boundary conditions based on experimental tests
- Results post processing: stress/strain loops & stabilised stress evolution to failure
- Hence we can use these results to elucidate Fatigue life difference

Stress distributions

## Crystal Plasticity Model

Based on multiplicative decomposition of the total deformation gradient:

$$F = \frac{\partial x}{\partial X} = F^e F^p$$

Octahedral and cubic slip systems control plastic deformation. For each slip system  $\alpha$ , shear strain rate is given by:

$$\dot{\gamma}^\alpha = \dot{\gamma}_0 \exp \left[ -\frac{F_0}{\kappa \theta} \left\langle 1 - \frac{|\tau^\alpha - B^\alpha| - S^\alpha \mu / \mu_0}{\hat{\tau}_0 \mu / \mu_0} \right\rangle^p \right]^q \text{sgn}(\tau^\alpha - B^\alpha)$$

$$\dot{B}^\alpha = h_B \dot{\gamma}^\alpha - r_D B^\alpha |\dot{\gamma}^\alpha|$$

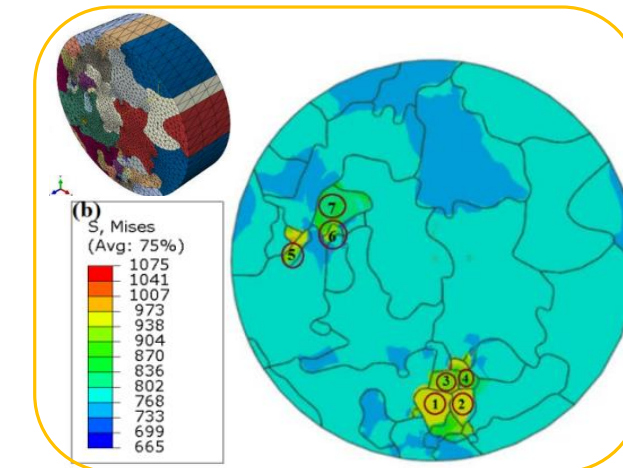
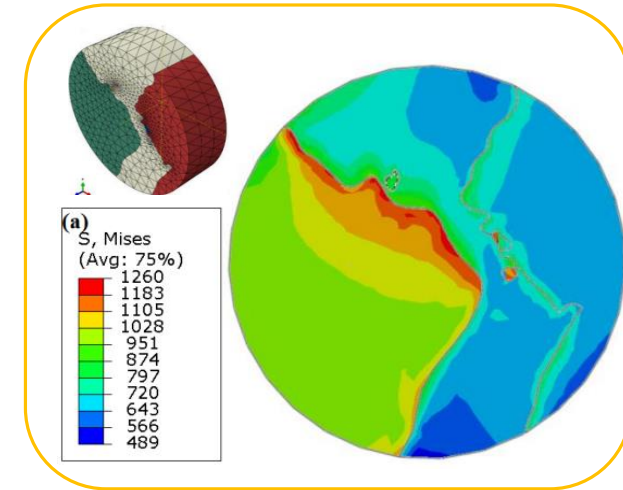
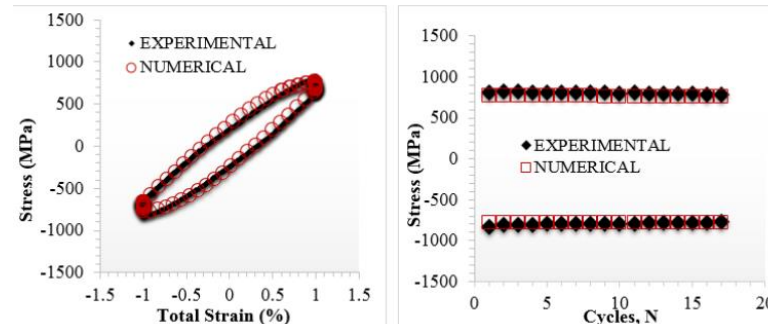
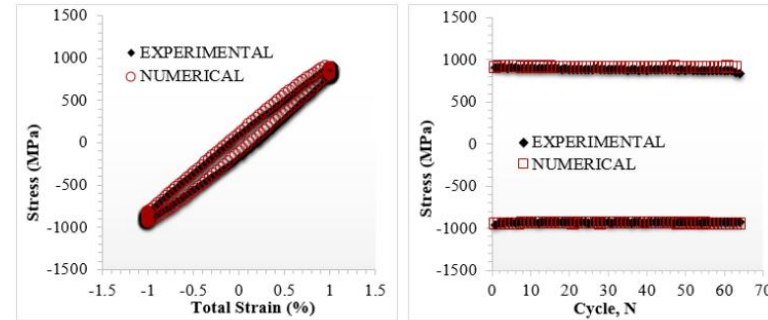
Back stress evolution

$$\dot{S}^\alpha = [h_S - d_D (S^\alpha - S_0^\alpha)] |\dot{\gamma}^\alpha|$$

Slip system resistance evolution

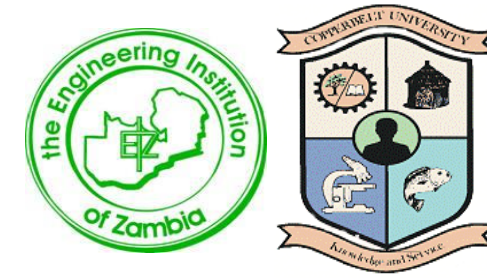
Finite element model implemented in ABAQUS as a UMAT, via Fortran

## Simulation vs test comparison

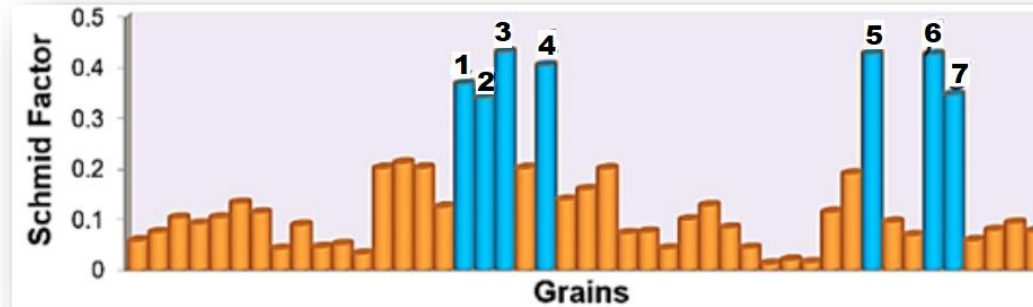
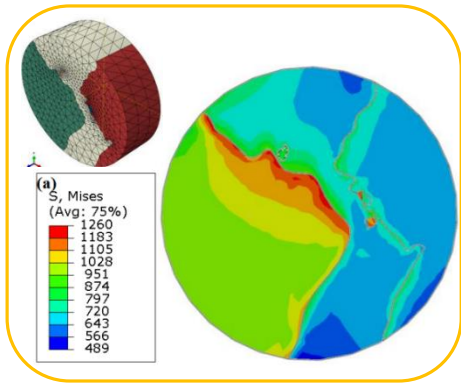




# FE modelling - ABAQUS

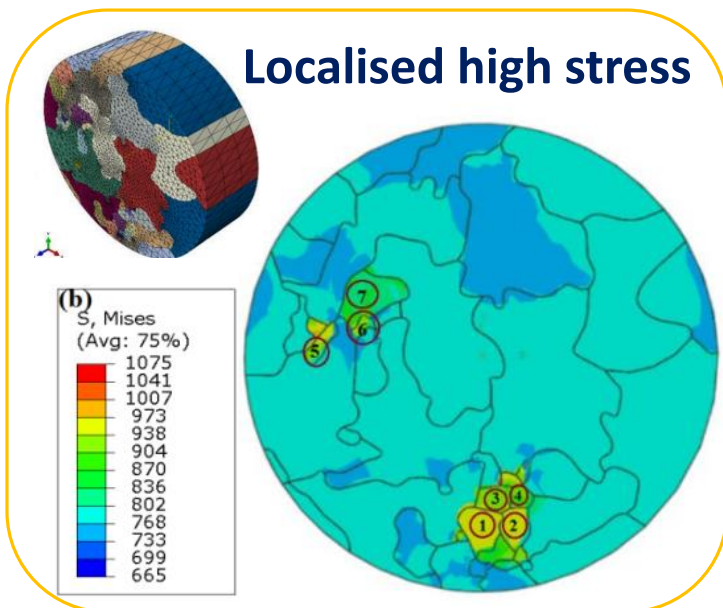


- Need to investigate localised high stress in model (b)
- Grains with high stress are numbered i.e., 1 - 7
- Orientations for all grains in model (b) was considered
- Based on the orientations, Schmid factors for each grain were calculated

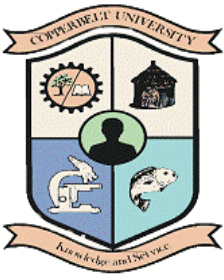


| Grain | $\phi_1$ (°) | $\Phi$ (°) | $\phi_2$ (°) | Schmid factor |
|-------|--------------|------------|--------------|---------------|
| 1     | 21.91        | 43.5       | 42.19        | 0.335184      |
| 2     | 38.63        | 41.27      | 40.85        | 0.324106      |
| 3     | 136.32       | 35.07      | 71.91        | 0.446824      |
| 4     | 125.45       | 31.87      | 68.97        | 0.418316      |
| 5     | 335.28       | 45.09      | 60.74        | 0.436073      |
| 6     | 61.26        | 33.58      | 73.57        | 0.441784      |
| 7     | 268.81       | 19.08      | 86.71        | 0.308274      |

- Since shear is proportional to Schmid factor
- The 7 grains yielded and failed before the rest
- Hence, this led to the reduced fatigue
- Failure was caused by misorientations generated at casting stage
- Such defects are normally common in engineering components



$$(\tau_{RSS}) = (\sigma) \underbrace{\sin \Phi \sin \phi_2 \cos \Phi}_{\text{Schmid factor}}$$



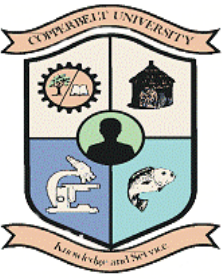
# Conclusions

- **Illustration of capability of FEM as a tool for solving existing and future (mechanics) engineering problems.**
- **Results were used to elucidate difference in LCF life**
- **Methodology can be applied to study other alloys**
- **Method is useful to solve other complex engineering problems, including:**
  - 1) Sheet metal forming deep- and cup-drawing,
  - 2) Extrusion and process/product design
  - 3) Failure due to mechanical and diffusion interaction

# Recommendations

- Since such tools are available for various engineering disciplines, local engineers need to be trained
- Investment in the state-of-the-art equipment and modern engineering software, in research centres.
- Continuous curricula review, to train engineers to innovatively solve local challenges in health, energy, agriculture, transport, and others.





*The End*

THANK YOU FOR YOUR ATTENTION.

