Accelerated crystal plasticity simulations for deformation behaviour of materials using machine learning

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INTRODUCTION

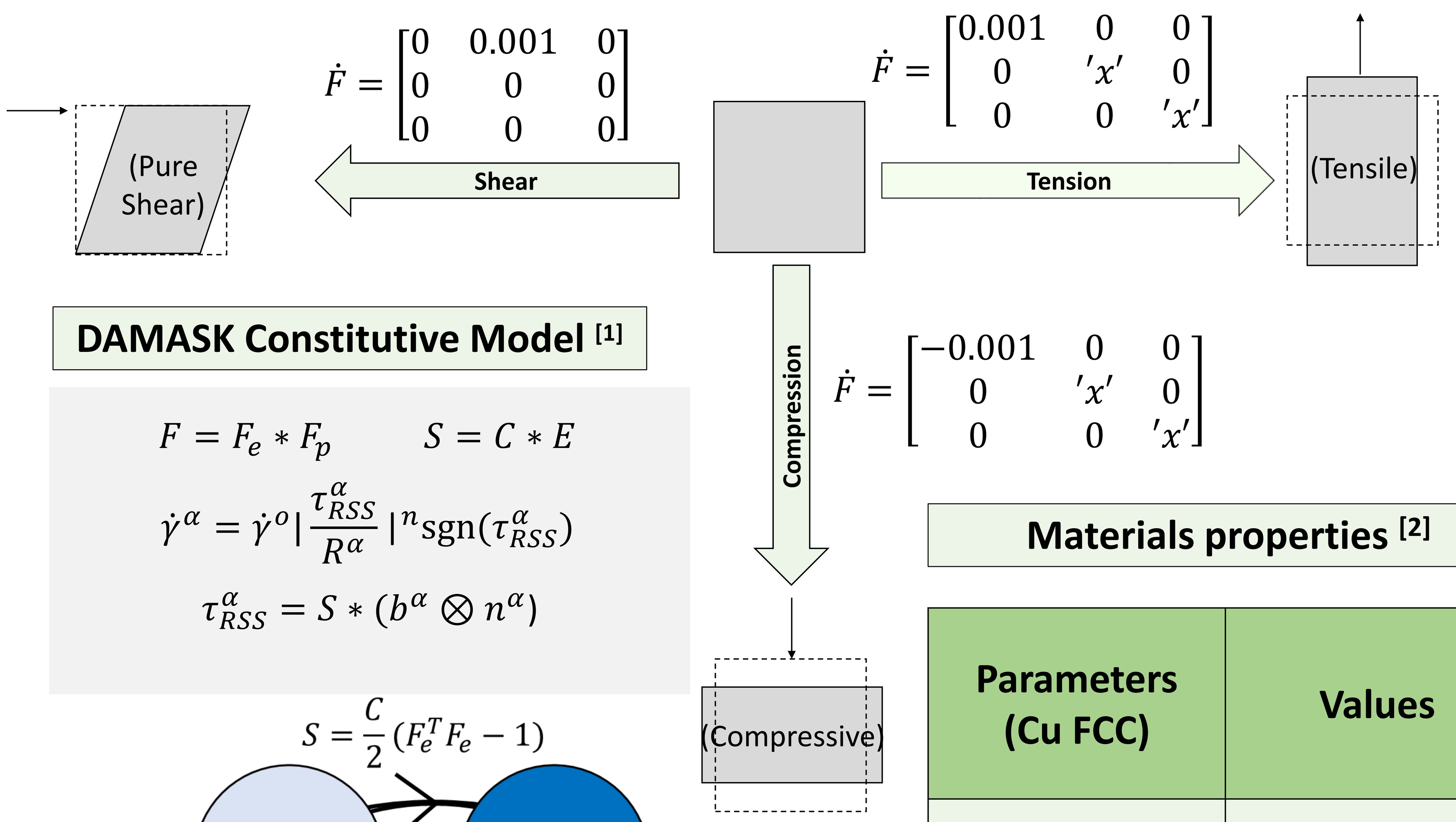
- **Crystal Plasticity Simulations →** Synthetically generated microstructures → Reduced time consumption and computational costs
- **Applications →** Advanced material designing, automobile, aerospace, microelectronics, biomedical and defence applications
- **Plasticity Simulation Techniques →** Finite Element Method, Phase Field Models, Boundary Element Method, Isogeometric Analysis

OBJECTIVE

- To study the pattern in the variation of the textural response parameters: Euler angles and Kernel Average Misorientation (KAM) values
- To predict the texture of the microstructure for extrapolated strain values using Machine Learning and Deep Learning models

METHODOLOGY

DREAM.3D	DAMASK	Machine Learning	ATEX
2D Synthetic microstructure (RVE) generation using DREAM.3D software	Microstructure deformation using Düsseldorf Advanced Material Simulation Kit (DAMASK)	Extrapolated texture prediction using Machine Learning (ML) models	Textural analysis using ATEX software

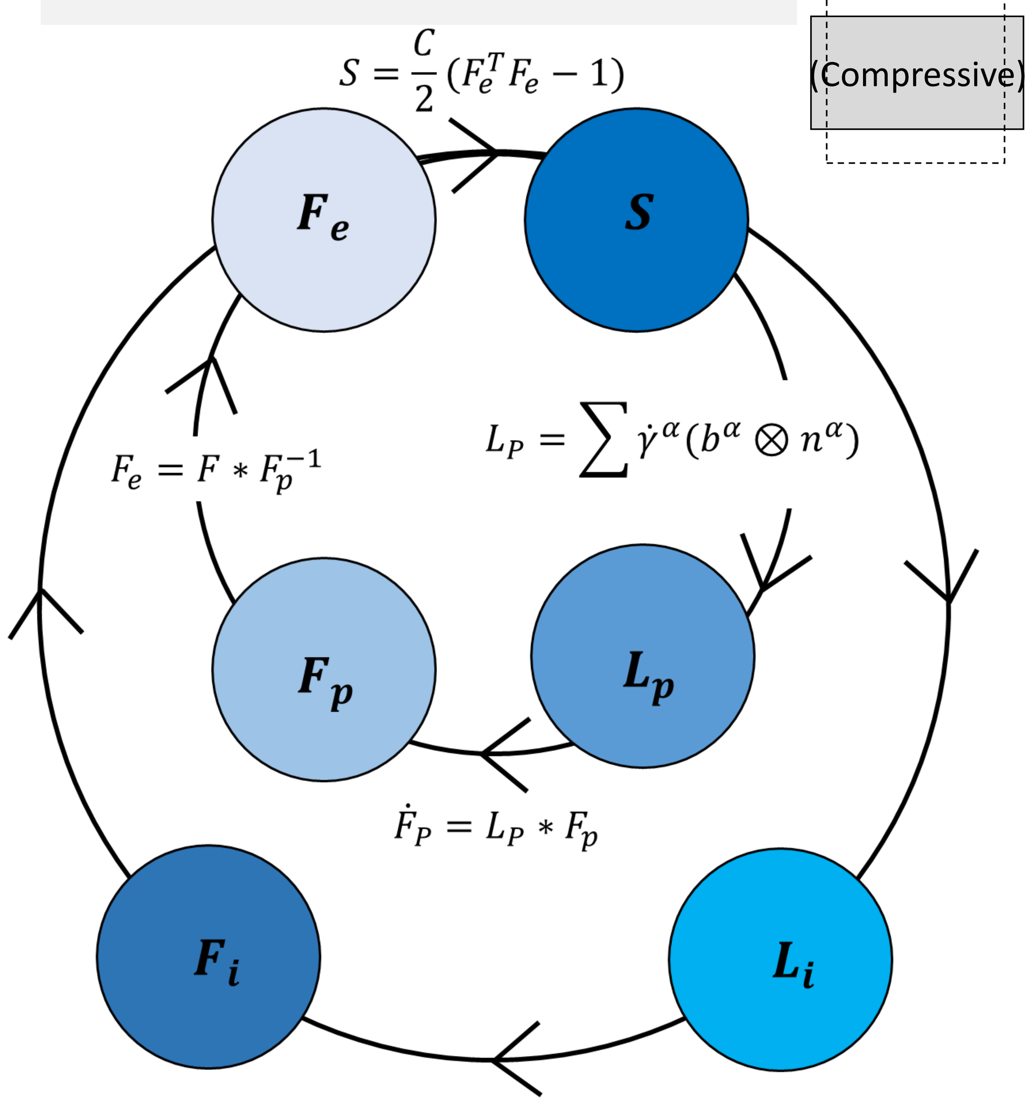


DAMASK Constitutive Model [1]

$$F = F_e * F_p \qquad S = C * E$$

$$\dot{\gamma}^{\alpha} = \dot{\gamma}^{o} \left| \frac{\tau^{\alpha}_{RSS}}{R^{\alpha}} \right|^{n} \mathrm{sgn}(\tau^{\alpha}_{RSS})$$

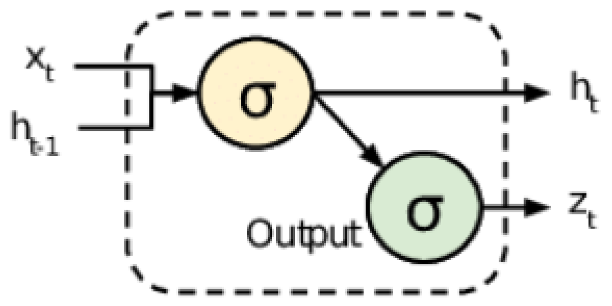
$$\tau^{\alpha}_{RSS} = S * (b^{\alpha} \otimes n^{\alpha})$$



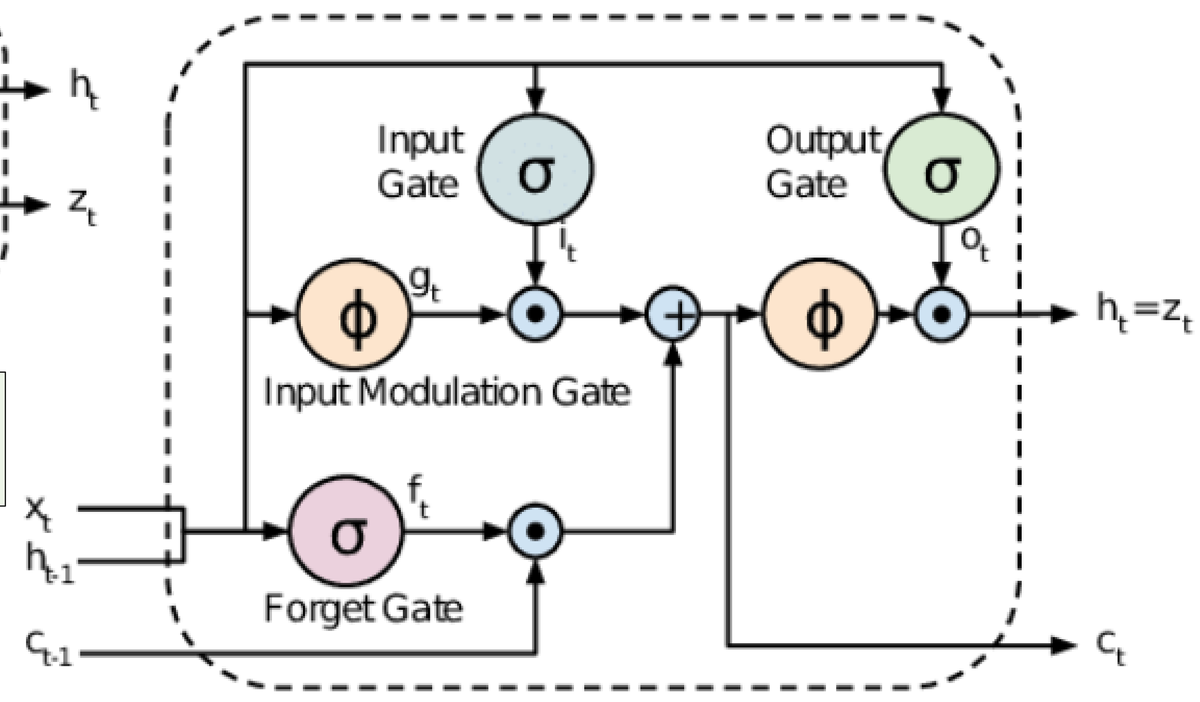
Materials properties [2]

Parameters (Cu FCC)	Values
C_{11}	168.6 GPa
C_{12}	121.50 GPa
C_{44}	75.59 GPa
R^{α}	240 MPa
τ^{α}_{RSS}	500 MPa
h_o	1
$h_{sl\text{-}sl}$	1.4
n	20
a	1

RNN Unit



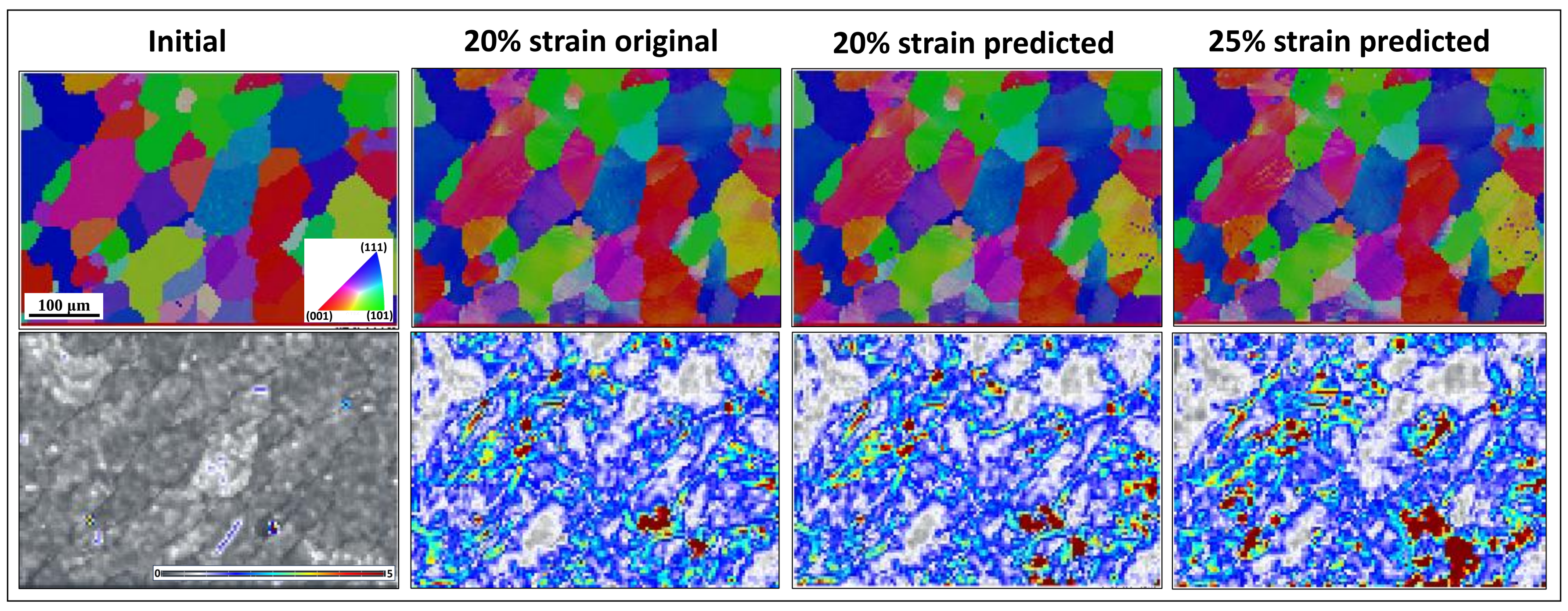
LSTM Unit



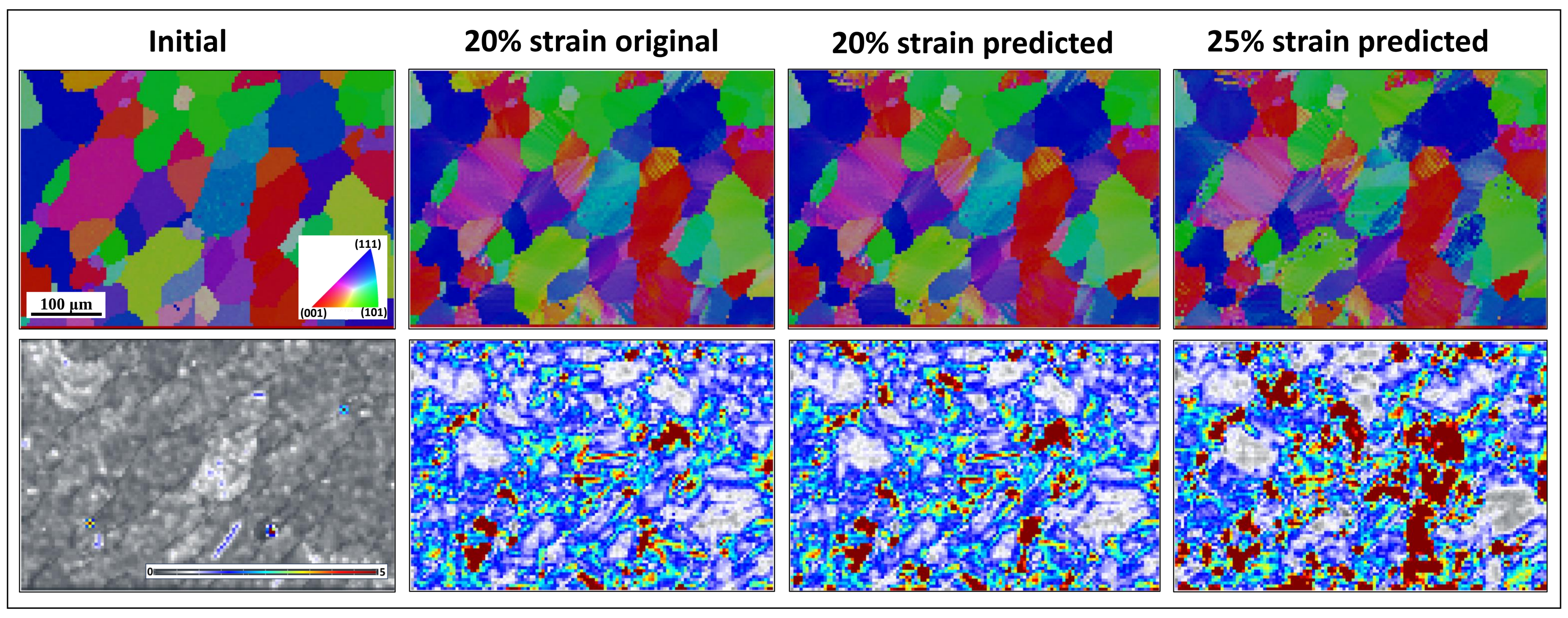
Long Short Term Memory (LSTM) Model

RESULTS

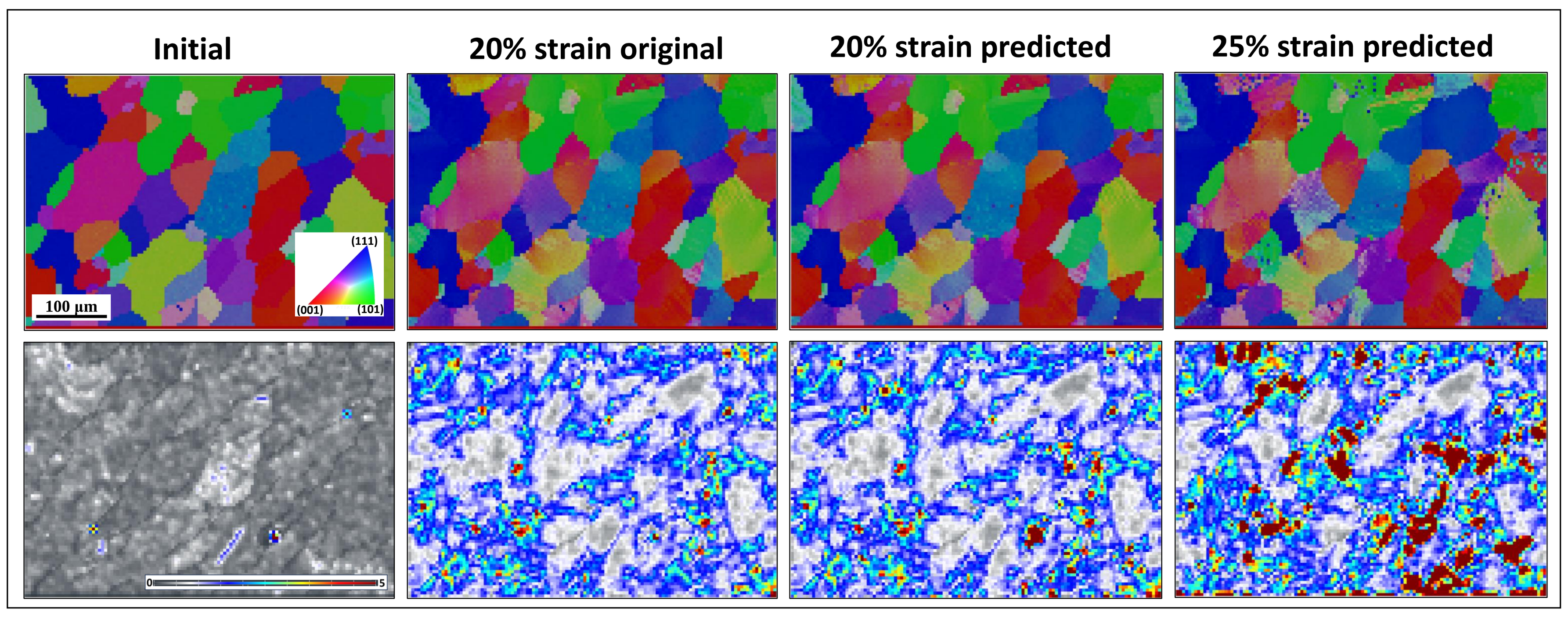
Tension



Compression



Shear



SUMMARY

- DAMASK simulations were used to generate microstructures with the applied strain values for a given stress state condition
- The texture evolution was successfully captured by the DAMASK simulated microstructure
- RNN-LSTM model was built and successfully trained using simulated microstructure to predict the texture response (Euler angles) for the final strain values
- The simulated and predicted microstructure shows a good match (Euler angles, KAM values)
- RNN-LSTM model accelerates the prediction of microstructure at further higher strains

FUTURE WORK

- To build classification models for the predicting the strain path that a given microstructure has been subjected to
- To incorporate stress concentration in the given microstructure in order to predict the failure strain value

REFERENCES

[1] F. Roters et. al., Comput. Mater. Sci.,158, 420-478, (2019)

[2] U.F. Kocks, Metall. Mater. Trans. B, 1, 1121-1143, (1975)

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