

An investigation into the effect of strain localisation on forged β -annealed Ti-6Al-4V.

Patrick Curran ^{1,a}, Pratheek Shanthraj ¹, Philip Prangnell ¹, Nicholas Byres ², Benjamin Dod ³, Michael Atkinson ¹, Adam Plowman ¹, Dongchen Hu ¹, João Quinta da Fonseca ¹.

¹University of Manchester, Manchester, United Kingdom, ²AIRBUS, Bristol, United Kingdom, ³AIRBUS, Toulouse, France, ^aPatrick.curran@manchester.ac.uk

Abstract

Accurate predictive models of fatigue life for aerospace components can offer weight reductions, improving the efficiency and decreasing the carbon footprint of air travel. Currently macroscopic experimental stress-strain data is used to find the CP input parameters. In this work we used high resolution digital image correlation (HRDIC) to microscopically validate a crystal plasticity (CP) model for strain localisation, as a precursor to fatigue crack initiation. We found that macroscopic calibration works for the elastic region but does not correctly predict the stress around the yield stress and that subsurface material does influence the response, although this is difficult to model. Once recalibrated, the CP modelling results will be used to predict fatigue initiation at the microstructural scale. These predictions will be compared to results from 4-point bend fatigue experiments.

Possible Sessions

2. Aerospace Applications, 13. Metal and Microstructures, 14. Model Validation

Introduction

Fatigue life estimation is an important part of safety assurance for aircraft manufacturers. Fatigue crack initiation in Ti-6Al-4V (Ti64) with bimodal microstructures is frequently associated with the presence of neighbouring soft-hard grains [1], meaning cracks form based on the local crystallography [2]. Similar mechanisms can also be seen in fully lamellar microstructures [3]. CP models use the orientations and neighbouring orientations of grains to predict the response, so researchers have used CP to predict fatigue crack initiation in Ti64 [4].

Crystal plasticity models are often calibrated by fitting the predicted macroscopic, polycrystal stress strain curve to experimental data [5]. However, for fatigue, it is essential that the models are validated at the relevant scale, i.e. at the microstructural scale. Recent advances in high resolution digital image correlation (HRDIC) make it possible to investigate slip activity at the nano scale, when combined with Electron Back Scatter Diffraction (EBSD). These measurements can be used to validate crystal plasticity predictions.

Method

Macroscopic calibration of a CP model for wrought β -annealed Ti64 was carried out by fitting the macroscopic true stress-strain response obtained via a standard tensile test, and using true stress-strain predictions from representative volume elements (VE) that included the texture of the material, and the phenomenological work hardening law which is implemented into DAMASK [6]. Parameters were initially drawn from literature and then changed iteratively until a good fit was obtained, results can be seen in table 1 macro-validated. In this model it was assumed that Ti64 has a single α -phase. The secondary β -phase, which accounts for $\approx 5\%$ of the volume, strengthens the material isotropically.

In-situ tensile testing was carried out using a TANIST in-situ testing system, which is a TESCAN Clara FEG-SEM equipped with an in-chamber integrated NewTec MT1000 5KN stress rig. Three regions of interest (ROI) were then selected, each covering an area of $500 \times 500 \mu\text{m}$. The HRDIC pattern had particles approximately 100nm in diameter, produced via vapour gold remodelling [7]. Images were taken every $50 \mu\text{m}$ of elongation up to $1000 \mu\text{m}$, or $\approx 4\%$ true strain. Data was processed in DaVis to calculate a deformation field, then passed to DefDap [8], a python package that linked the deformation fields to EBSD data to measure strain localisation and slip activity.

The same EBSD map used in the HRDIC experiment was imported into a 2D representative VE, which was extruded to create a 2.5D model. The CP simulations were strain controlled and used the simulation framework MatFlow [9] which links together DefDap and DAMASK, a crystal plasticity modelling package. CP cannot predict dislocation slip like seen in HRDIC, therefore grain averaged strains were taken for a direct comparison between HRDIC and CP.

Result

The predicted stress-strain curves for the 3 regions, shown in Fig 1a, shows a good comparison between the HRDIC and CP before yield and at higher strains. Around the yield stress the predictions are less accurate, especially in ROI2, suggesting that the input yield stress is too high in the CP model. The experimental stress-strain gradients during plastic deformation are higher than those from the simulations, suggesting that the CP parameters for work hardening are too low.

The strain-strain comparison shown in Fig 1b, shows below the elastic limit there is a good match between CP and HRDIC with the average value falling close to the theoretically best fit line. After the elastic limit the mean grain average effective shear strain (ESS) fall within $\pm 25\%$ of the theoretical best fit line. Additionally, the standard deviation falls on the theoretical best fit line, suggesting that the spread is within an acceptable range.

After deformation ROI1 was re-polished so that $20 \mu\text{m}$ of material was removed. Then ROI1 was re-EBSD, which showed that the hard surface grains had been removed. As the CP took surface orientations

and extruded them out of plane, it did not account for subsurface soft orientated grains. So, the CP predicted ROI1 to be harder than experimentally measured, this can be seen in Fig 1b, where the blue series is to the right of the best fit line. HRDIC was analysed as a time series and looked for the onset of slip activity relative to the engineering stress. This can then be used to approximately measure the critically resolved shear stress (CRSS) and can be seen in table 1. These measured values were approximately half that measured from macroscopic calibration. Additionally, we found that what appears to be pyramidal $\langle a \rangle$ type slip. In the future the model needs to be rerun to include pyramidal $\langle a \rangle$ type slip and the lower CRSS values, the work hardening rate needs to be increased so the macroscopic stress-strain curve still fits.

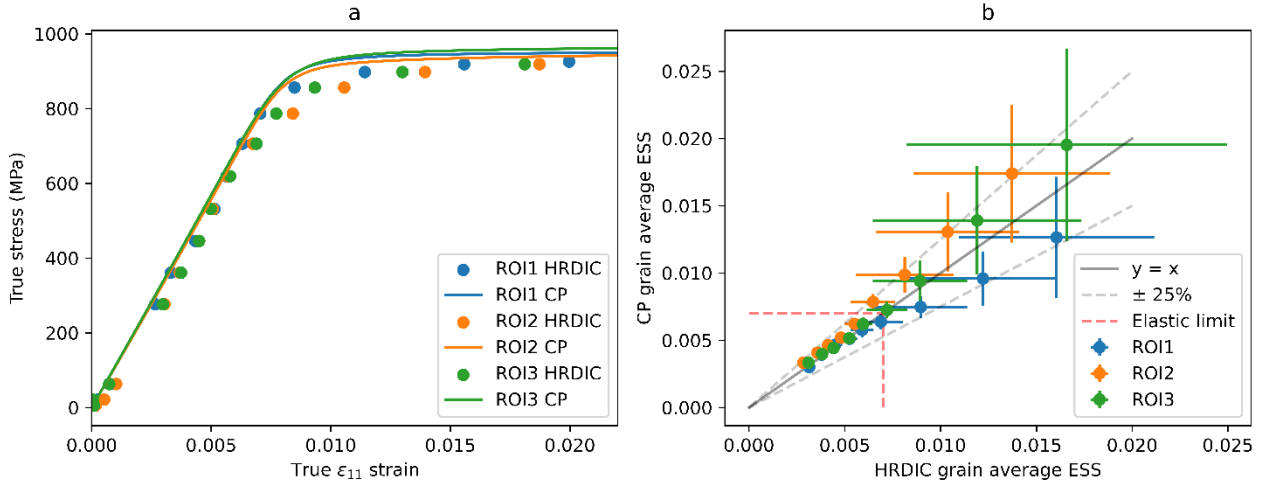


Fig 1a: Predicted stress-strain curve using macroscopically validated parameters up to 2% ϵ_{11} strain (strain parallel to the applied load). Figure 1b: Compares grain average effective shear strain (ESS) between CP simulations and HRDIC experiments up to 2% ϵ_{11} strain. Each cross represents an imaging step, low strain level imaging has been excluded due to computational memory limits. The mean grain average ESS is the centre of the cross and the length of the cross is equal to the standard deviation. The $y=x$ line is plotted as the theoretical best fit with a $\pm 25\%$ around $y=x$ to show the spread of values.

Slip System	Marco-validated CRSS [MPa]	Micro-validated CRSS [MPa]	Literature[10] [MPa]
Basal	400	239	330
Prismatic	420	214	396
Pyramidal $\langle a \rangle$	n/a	328	n/a
Pyramidal $\langle a+c \rangle$	612	270	561

Table 1: CRSS values from different methods.

Conclusion

Macroscopic validation provides a non-unique set of input parameters for CP modelling. At stresses lower than the yield stress, the prediction is accurate. As the computational material starts to yield the non-unique parameters means the simulated response is likely to differ from the physical response. HRDIC offers a way to check the accuracy of the parameters and also uniquely measure the CRSS of specific slip systems which can then be used to generate better predictions.

References

- [1] I. Bantounas, T. C. Lindley, D. Rugg, and D. Dye, "Effect of microtexture on fatigue cracking in Ti-6Al-4V," *Acta Mater.*, vol. 55, no. 16, pp. 5655–5665, 2007, doi: 10.1016/j.actamat.2007.06.034.
- [2] F. P. E. Dunne, A. Walker, and D. Rugg, "A systematic study of hcp crystal orientation and morphology effects in polycrystal deformation and fatigue," *Proc. R. Soc. A Math. Phys. Eng. Sci.*, vol. 463, no. 2082, pp. 1467–1489, 2007, doi: 10.1098/rspa.2007.1833.
- [3] A. L. Pilchak, R. E. A. Williams, and J. C. Williams, "Crystallography of fatigue crack initiation and growth in fully lamellar Ti-6Al-4V," *Metall. Mater. Trans. A Phys. Metall. Mater. Sci.*, vol. 41, no. 1, pp. 106–124, 2010, doi: 10.1007/s11661-009-0064-2.
- [4] D. L. McDowell and F. Dunne, "Microstructure-sensitive computational modeling of fatigue crack formation," *Int. J. Fatigue*, vol. 32, no. 9, pp. 1521–1542, 2010, doi: 10.1016/j.ijfatigue.2010.01.003.
- [5] K. Kapoor, R. Noraas, V. Seetharaman, and M. D. Sangid, "Modeling Strain Localization in Microtextured Regions in a Titanium Alloy: Ti-6Al-4V," *Integr. Mater. Manuf. Innov.*, vol. 8, no. 4, pp. 455–467, 2019, doi: 10.1007/s40192-019-00159-y.
- [6] F. Roters *et al.*, "DAMASK – The Düsseldorf Advanced Material Simulation Kit for modeling multi-physics crystal plasticity, thermal, and damage phenomena from the single crystal up to the component scale," *Comput. Mater. Sci.*, vol. 158, no. April 2018, pp. 420–478, 2019, doi: 10.1016/j.commatsci.2018.04.030.
- [7] F. Di Gioacchino and J. Quinta da Fonseca, "Plastic Strain Mapping with Sub-micron Resolution Using Digital Image Correlation," *Exp. Mech.*, vol. 53, no. 5, pp. 743–754, Jun. 2013, doi: 10.1007/s11340-012-9685-2.
- [8] M. Atkinson, R. Thomas, A. Harte, P. Crowther, and J. Quinta da Fonseca, "DefDAP: Deformation Data Analysis in Python." 2021, [Online]. Available: <https://zenodo.org/record/4697260/export/json#.YO68kehKg2w>.
- [9] A. Plowman, "MatFlow." 2021, [Online]. Available: <https://pypi.org/project/matflow/>.
- [10] P. Dawson, D. E. Boyce, J. S. Park, E. Wielewski, and M. P. Miller, "Determining the strengths of HCP slip systems using harmonic analyses of lattice strain distributions," *Acta Mater.*, vol. 144, pp. 92–106, 2018, doi: 10.1016/j.actamat.2017.10.032.