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A 3D single-crystal hyperelastic-viscoplastic material model, applied to metallic HCP granular structures

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ABSTRACT

In the aviation industry, high strain rate deformation can occur during bird strike or events associated with engine failure such as fan blade detachment. Understanding the material flow behaviour and deformation mechanisms active at high strain rates will allow both microstructural and chemical optimisation of candidate alloys

An explicit hyperelastic-viscoplastic single-crystal rate dependent material model is outlined for use with HCP granular structures such as titanium. The material model allows for slip on all of the thirty slip systems present in the HCP crystal[1]. Crystallographic orientation is controlled through the input of Euler angles which in turn defines the initial slip system configuration. Each of the five families of slip systems can have specific material properties assigned to them.

To form an accurate simulation of the granular microstructure the geometry of the sample needs to be considered. Two and three dimensional Representative Volume Elements (RVE's) are created through the use of NEPER and Gmsh. These RVE's are based on data provided from Electron Backscatter diffraction (EBSD) of Ti-6Al-4V.

A single element plane strain case is outlined and compares the results between the original 2 dimensional code and the new three dimensional model. The simulation compares the XY, XZ, and YZ orientations of the three dimensional case to the XY plane of the two dimensional case, resulting in a relative error of zero.

Keywords: *Crystal viscoplasticity; HCP crystals; titanium modelling*

1. Introduction

Aero engine manufacturers face the problem of designing components for high strain rate scenarios such as bird strike, while at the same time trying to reduce the weight of the components. Materials that exhibit high strength to weight ratios such as titanium are therefore a logical choice. Gaining a more in depth understanding of titanium's microstructure can help to develop the material's properties on a macro scale.

In Ti-6Al-4V the alpha phase is the predominant phase within the microstructure, this alpha phase has a HCP crystal structure. In plastic deformation slip can occur on any or all of the thirty slip systems that are present within the crystal. These thirty slip systems fit into five slip families as seen in figure 1 [1], each of these five families has its own Critical Resolved Shear Stress (CRSS) which govern the point of slip.

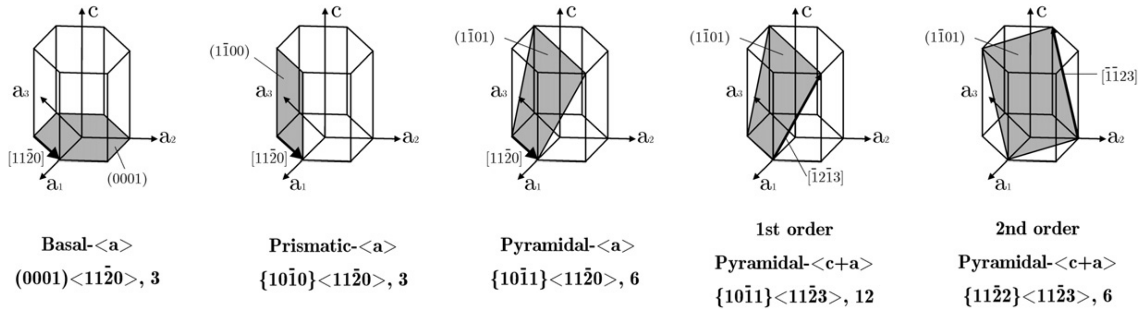

Figure 1: HCP Slip planes.

A two dimensional hyperelastic-viscoplastic material model has been adapted to form a three dimensional HCP crystal stress update routine with strain rate sensitivity. EBSD is used to gain micro structural data to inform the creation of RVE's. These RVE's can then be meshed and used in a finite element environment.

When completed, this model will allow an insight into the micro scale deformations which are difficult to observe in reality, thus giving a deeper understanding of the deformation characteristics of the material.

2. Material model

The model outlined is based on the multiplicative split of the deformation gradient as seen in equation 1; this is then coupled with a compressible Neo-Hookean description of the elastic region. This is paired with a viscoplastic model to provide a hyperelastic-viscoplastic explicit stress update routine. A brief description of the model is given here, for the full model see [2].

$$\boldsymbol{F} = \boldsymbol{F}^e \boldsymbol{F}^p \tag{1}$$

The compressible Neo-Hookean hyperelastic law is used to govern the reversible behaviour of the material, with the stresses being found through the use of the hyperelastic potential. The advantage of using the compressible Neo-Hookean is that it leads to a simple format for the return mapping equations originally proposed by Miehe [3][4]. Other elastic laws could be used but due to metals having small elastic distortions this would lead to having little effect upon the numerical results [2].

To have a multi-surface definition for the yield criterion it is necessary to split the physical slip surface of the crystal into mirrored parts. This means having 60 slip systems in the HCP crystal. The setting of these slip systems for HCP crystals has been added to the model proposed by de Souza Neto [2] along with the expansion to three dimensions. Each family of slip systems in the HCP crystal has an individual CRSS value which allows for the formulations of the yield surfaces as shown in equation 2 [2].

$$\boldsymbol{\Phi}^{\alpha}\left(\tau^{\alpha}, \tau_y^{\alpha}\right) \equiv \tau^{\alpha} - \tau_y^{\alpha}, \quad \alpha = 1, \dots, 2n_{syst} \tag{2}$$

Where τ_y^{α} is the CRSS for slip system α. If hardening is present then the CRSS value of the slip system α depends on the history of the deformation. In this work a linear hardening law is adopted to govern the evolution of the CRSS value of each slip system. τ^{α} is the Schmid resolved shear stress in the slip system α [2].

The rate of deformation can have significant effects on the mechanics of the material, especially in metals, therefore a suitable slip rate law is needed. In this work the Perić slip rate law is used and can be seen in equation 3 [2].

$$\dot{\gamma}^{\alpha} = \begin{cases} \frac{1}{\mu}\left[\left(\frac{|\tau^{\alpha}|}{\tau_y}\right)^{1/\epsilon} - 1\right] & if\ \boldsymbol{\Phi}^{\alpha}(\tau^{\alpha}, \tau_y^{\alpha}) \geq 0 \\ 0 & if\ \boldsymbol{\Phi}^{\alpha}(\tau^{\alpha}, \tau_y^{\alpha}) < 0 \end{cases} \tag{3}$$

The constants μ and ϵ are the viscosity and rate-sensitivity parameters respectively. An exponential map based integration algorithm combined with a local Newton Raphson algorithm is used to calculate the stresses.

3. Titanium grain structure

An EBSD data set for Equiaxed Ti-6AL-4V is provided by Timet UK. The EBSD map shown in figure 2 is the result of this analysis. The EBSD data also provides orientations of the grains in terms of Euler angles, along with grain size information.

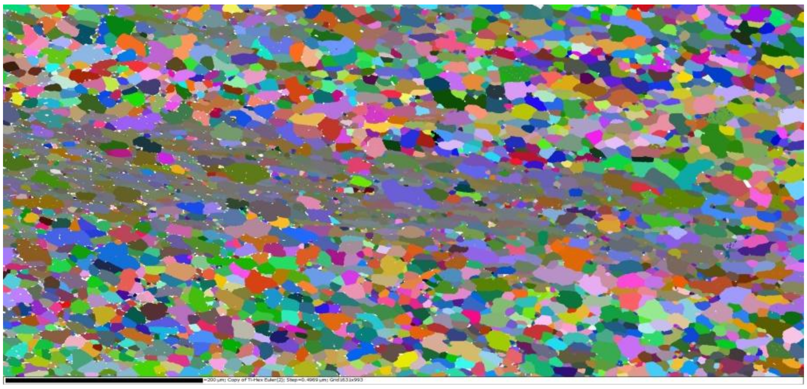

Figure 2: Ti-6Al-4V EBSD map.

This data is then used to help create Representative Volume Elements (RVE's) for simulations. To create the RVE's an open source program called NEPER is used, which uses Voronoi tessellations to create the grain structures. A more in depth explanation of NEPER can be seen in [5]. Statistics for the created RVE can also be outputted, which allows for cross checking. This ensures that the statistical grain size of the RVE and the EBSD data match. This, however, does not check for a geometrical match of the microstructure, therefore features such as macrozones are currently not captured. Figure 3 shows two dimensional and three dimensional RVE's created from the EBSD data. The statistical data from the created RVE's matched well with the average grain size in the EBSD data.

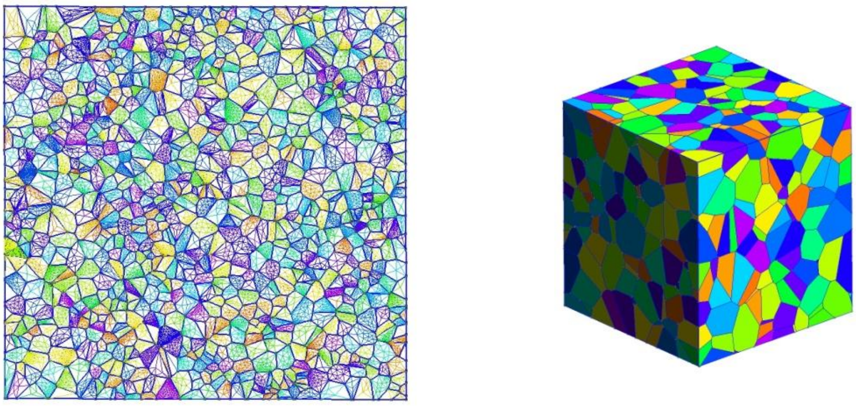

Figure 3: Two dimensional and three dimensional RVE's created from NEPER.

The grain geometries that are created by NEPER are then meshed in Gmsh, with each grain being seen as a volume. This allows each of the grains to have material parameters associated to it.

4. Elastic tests

A single element is constrained so that all nodes are fully defined to provide a plane strain case. The three dimensional case is compared to the already existing two dimensional code. A 0.1 (10%)tensile displacement is then applied. A bulk and shear modulus are prescribed as 106.4GPa and 43.9GPa respectively. The simulation is run for 100 increments of equal size. The comparison of results between the original two dimensional code and the three dimensional code are given in table 1. It can be seen in the table that there is no difference between the two codes.

The three dimensional cube is also tested on the different faces (XY, XZ, YZ) with the same properties as before, the values of the results for each of these faces matches each other and the original two dimensional code.

Table 1: Stresses obtained from elastic testing of a single element.

	XX (GPa)	YY (GPa)	ZZ (GPa)
2D code	15.11	6.89	6.89
3D Code	15.11	6.89	6.89
Relative error	0.00	0.00	0.00

5. Conclusions

An outline of the material model has been presented, this model allows for the material parameters to be specified for each of the five families of slip systems. EBSD data has been used to inform the creation of RVE’s that can capture the nature of titanium microstructures.

Tests on single element plane strain case of the elastic deformation have been carried out and compared to the original two dimensional code which has been validated in [2]. It can be seen that there is no difference between the two codes with the relative error being zero.

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