Implementation of a unified material model in finite element analysis and simulations of cracked components

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Abstract

A new form of a unified viscoplastic material model based on overstress was implemented in finite element code using a material constitutive equation programme. The analysis results, employing equivalent forms of the stresses, the overstresses and the inelastic strains, were consistent with results obtained from: (i) uniaxial direct rate dependent integration simulations, (ii) results obtained indirectly by employing experimental stress strain curves and, (iii) experiments. Simulations of two batches of CP (commercial purity) titanium specimens containing cracks subjected to either different displacement rates, or sustained loads (creep) predicted material deformation and failure behaviour that was close to experimental results. However, the simulation results were dependent on material constants that were difficult to determine experimentally.

Introduction

Components’ failure at room temperature due to sustained load cracking and time dependent ductile tearing have long been recognised e.g. Jordan and Freed\(^{4}\), Reed-Hill\(^{2}\) and Hartley and Duffy.\(^{3}\) More recently, Smith and Jones\(^{4,5}\) investigated the strain-rate sensitivity and sustained load deformation at room temperature of commercial purity (CP) titanium. It was shown that the uniaxial rate dependent deformation of the CP titanium at room temperature was well...
described by using a visco-plastic overstress model developed by Cernocky and Krempl, Figure 1. The Cernocky-Krempl model, generically termed a unified elastic-viscoplastic model, was particularly suitable for the CP titanium simulations since deformation and cracking due to rate-dependent plastic flow, sustained load and stress relaxation were described in one set of equations. However, the fracture behaviour could not be fully explained from a uniaxial model and further numerical simulations using finite element analysis were required.\textsuperscript{5}

In the past, considerable efforts have been made to implement the Krempl-Cernocky model in Finite Element (FE) programmes. For example, Little, Krempl and Shih\textsuperscript{7} generalised the uniaxial overstress model to the multiaxial state by introducing an overstress invariant and solving the numerically stiff equation by a forward gradient method. They simulated loading rate sensitivity in cracked specimens of type 304 stainless under small scale yielding (SSY). Later, Nishiguchi, Sham and Krempl\textsuperscript{8} further developed the overstress model to include finite deformation behaviour. Sham and Chaw\textsuperscript{9} implemented this extended model in a finite element programme using a displacement-based incremental procedure.

In the current work a simplified numerical procedure has been developed, which enabled the implementation of the unified viscoplastic equations in a commercial FE code (ABAQUS) employing a user material subroutine (UMAT). Verifications of the FE material model were carried out using simple uniaxial and 2D analyses and, subsequently, the model was used to predict the mechanical behaviour of a cracked component (a compact tension (CT) specimen). The CT specimen simulations were compared with results obtained from an extensive experimental programme, carried out at room temperature with two batches of the CP titanium.\textsuperscript{10-12} Experimental results obtained with the CT specimens are shown in Figure 2 for two load point displacement rates.

**Material constitutive equations**

Smith and Jones\textsuperscript{4} demonstrated that the CP titanium post-elastic deformation response is strain rate sensitive, and for a given constant strain rate a unique uniaxial stress-strain curve is obtained. If the strain rate is suddenly changed the subsequent stress strain curve matches the curve for the new strain rate, Figure 1. The uniaxial deformation response was well described by a single, non-linear differential equation, where the total strain rate \( \dot{\varepsilon} \) is given by:

\[
\dot{\varepsilon} = \dot{\varepsilon}^e + \dot{\varepsilon}^in
\]

where \( \dot{\varepsilon}^e \) is the elastic strain rate, \( \sigma / E, E \) is the modulus of elasticity and \( \dot{\varepsilon}^in \) is the inelastic strain rate, given by:

\[
\dot{\varepsilon}^in = \frac{\Sigma}{E k[\Sigma]}
\]
Where the relaxation function, $k[\Sigma]$, is defined as a function of the overstress $\Sigma$, the stress that exceeds an "equilibrium" stress-strain curve, described by the function $g[\epsilon]$, so that

$$\Sigma = \sigma - g[\epsilon]$$  \hspace{1cm} (3)

A simple generalisation of the overstress model for the general case of stress and strain is introduced by using equivalent values for the stress ($\sigma_{eq}$), "equilibrium" stress ($g_{eq}$), total strain ($\epsilon_{eq}$) and the total strain increment ($\Delta\epsilon_{eq}$) as follows:

$$\sigma_{eq} = \sqrt{\frac{3}{2}} S_{ij} S_{ij} \hspace{1cm} (4)$$

$$g_{eq} = \sqrt{\frac{3}{2}} g_{ij} g_{ij} \hspace{1cm} (5)$$

$$\epsilon_{eq} = \sqrt{\frac{2}{3}} \epsilon_{ij} \epsilon_{ij} \hspace{1cm} (6)$$

$$\Delta\epsilon_{eq} = \sqrt{\frac{2}{3}} \Delta\epsilon_{ij} \Delta\epsilon_{ij} \hspace{1cm} (7)$$

where $S_{ij}$ and $\epsilon_{ij}$ are the deviatoric components of the stress and strain tensors respectively.

Substitution of eqns. 4, 5, 6 and 7 in eqns. 1, 2 and 3 a generalised form of the overstress constitutive material model is:

$$\dot{\epsilon}_{eq}^{\text{total}} = \dot{\epsilon}_{eq}^{\text{el}} + \dot{\epsilon}_{eq}^{\text{in}} \hspace{1cm} (8)$$

Where:

$$\dot{\epsilon}_{eq}^{\text{el}} = \frac{\dot{\sigma}_{eq}^{\text{el}}}{E} \hspace{1cm} \text{and}, \hspace{1cm} \dot{\epsilon}_{eq}^{\text{in}} = \frac{\Sigma_{eq}}{E k_{eq} [\Sigma_{eq}]} \hspace{1cm} (9)$$

and the equivalent overstress is:

$$\Sigma_{eq} = \sigma_{eq} - g_{eq}[\epsilon_{eq}] \hspace{1cm} (10)$$

To overcome the numerically 'stiff' equations, a forward gradient method developed by Argyris, Vaz and William\textsuperscript{13}, was employed using a weighting factor ($\theta$), as follows:

$$\Delta\epsilon_{eq}[t + \Delta t] = \Delta t\left[(1 - \theta) \dot{\epsilon}_{eq}^{\text{in}}[t] + \theta \dot{\epsilon}_{eq}^{\text{in}}[t + \Delta t]\right] \hspace{1cm} (11)$$

where \(0 \leq \theta \leq 1\).
A truncated Taylor expansion of the inelastic equivalent strain can be described as:

\[
\dot{\varepsilon}^{\text{eq}}_{\text{t}}[t + \Delta t] = \dot{\varepsilon}^{\text{eq}}_{\text{t}}[t] + \frac{\partial \dot{\varepsilon}^{\text{eq}}_{\text{t}}}{\partial \sigma} \Delta \sigma^{\text{eq}}_{\text{t}}[t + \Delta t] + \frac{\partial \dot{\varepsilon}^{\text{eq}}_{\text{t}}}{\partial \varepsilon} \Delta \varepsilon^{\text{total}}_{\text{eq}}[t + \Delta t]
\]

Rearranging eqn. (12), a new equivalent stress increment, \(\Delta \sigma^{\text{eq}}_{\text{t}}[t + \Delta t]\), is determined.

To calculate the inelastic strain increment matrix we assume proportional loading and use the Prandtl-Reuss relation of total deformation theory:

\[
\Delta \varepsilon^{\text{in}}_{ij}[t + \Delta t] = \frac{3}{2} \frac{\Delta \varepsilon^{\text{eq}}_{\text{t}}[t + \Delta t]}{\sigma^{\text{eq}}_{\text{t}}[t]} s_{ij}[t]
\]

Finally, the differences between the total strain increments and the inelastic strain increments are used to obtain stress increments from the generalised Hooke's law equations. The stress components are updated and the solution returns to the main FE code.

**Finite Element solution procedure**

The FE code requires updated, true (Cauchy) stress and the Jacobian matrix for each increment and for each material integration point. The visco-plastic model described above was coded into a subroutine, using the procedure shown in Figure 3. At each load step, after calling the material programme, the standard FE convergence routine was employed. The calculation of the material Jacobian \((\partial \sigma_{ij}/\partial \varepsilon_{kl})\) for every integration point was carried out assuming elastic constitutive stress-strain relationships throughout the analysis. Separate programmes were used for plane stress and plane strain conditions.

In general, the convergence rate of the simulations was more sensitive to time steps length at the slow strain rates of under \(10^{-4}\) s\(^{-1}\). This was a direct result of the numerical integration of equation (1). For the same number of time steps, an increase in time step length is required in order to maintain the same inelastic strain in a lower strain rate in comparison to a higher strain rate.

**Verifications of the FE model**

To undertake simulations of material behaviour the material constants in the constitutive equations were identified for the CP titanium from uniaxial tests at room temperature.\(^4,11\) Two different batches of material (ASTM B381) were considered, having equivalent oxygen contents of 14% and 19%, where the equivalent oxygen content (Oeq) is defined as:

\[
O_{\text{eq}} = \frac{1}{2} (O_2) + 2(N_2) + 0.75 (C) \quad \text{All in Wt/\%}
\]

\(14\)
Initial uniaxial FE simulations were found to be in excellent agreement with results using a programme to solve differential equations (SIMNON). Three loading conditions were examined using a simple uniaxial model consisting of 2 nodes in a single, one degree of freedom element.

**Simulations of cracked components**

The viscoplastic FE model was applied to a compact tension (CT) specimen, simulating the behaviour of a component containing a crack. The specimen dimensions were selected to match those used in an experimental programme on rate-dependent ductile crack growth in CP titanium. Due to symmetry, a 2-D model of one half of the CT specimen was constructed using a focused mesh at the crack tip. The specimen was constrained along the ligament and displacement was applied at the crack load point. The mesh near the crack tip had mid-side nodes at quarter distance in order to obtain the tip stress field distribution.

Previous rate-dependent simulations of CP titanium fracture have used a simple indirect method. For a given strain rate the stress strain response was obtained by numerical integration of eqn. (1). A range of stress strain curves were used in the indirect FE analyses to simulate a range of compact tension (CT) specimen load point displacement (lpd) rates. Figures 3, a-d compare simulations using the simple indirect strain rate method with those using the directly applied displacement rates, for two displacement rates and assuming plane strain or plane stress conditions. Good agreement is obtained irrespective of the applied displacement rate or whether plane stress or plane strain conditions are used.

To match the test conditions of the experimental programme, the FE model was subjected to different displacement rates at the initial crack length corresponding to experiments, Figure 2. The experimental results were generally bounded by the plane strain and plane stress FE simulations as shown in Figure 2, and it is notable that a good agreement exists between the average of the plane stress and plane strain FE results and the experimental results.

The sustained load (creep) behaviour of the CP titanium CT specimens was simulated by first applying a constant load rate up to the required level and, then keeping this load constant over a period of time. Material fracture was not directly simulated in the FE analysis. Instead, crack growth was considered by post-processing simulations using different crack lengths.

**Discussion and Concluding Comments**

A simplified form of over-stress visco-plastic material model, which employs equivalent values of stresses and strains, was used in commercial FE code to simulate time dependent fracture of CP titanium in room temperature, assuming proportional loading. The FE model was applied to a simple cracked component assuming plane strain or plane stress conditions. The component numerical simulation predictions of time dependent inelastic material deformations and cracking compared well with previous indirectly applied, time-dependent simulations and, more importantly, with experimental results for two batches of CP titanium.
Further analysis compared the visco-plastic model simulations to an existing rate-dependent material option in the FE code: the Malvern flow rule model. This analysis results have shown that the flow rule model overestimated the CP titanium material stresses at high rates due to the exponential relationship between the plastic strain rate and the applied stress. The differences between the two material models are demonstrated in Figure 4. The simulations give approximately the same results at the slower displacement rate of 10^{-4} mm/s, Figures 4a and 4b. However, at a higher rate of 1 mm/s the flow rule model simulations predicted much higher loads than did the overstress model for a given global displacement, Figures 4c and 4d.

It has been proposed previously, that the unified visco-plastic overstress model could be utilised to predict the rate dependent response of CP titanium material using one set of material functions. It was argued that a single test could provide all the material information required. This approach was demonstrated by numerical simulations of relaxation, creep, constant strain rate and constant stress tests. One main function in these models is an equilibrium curve which is independent of the loading path and test conditions. For the 14% Oeq material, it was also shown that a very similar stress strain curve was obtained under a slow strain rate tests (10^{-7} s^{-1}) when compared to loci of points from the relaxation tests. It was therefore proposed that since the equilibrium curve provided a limit below which no further deformation took place, the stress-strain creep curve could not cross this relaxed curve.

However, the uniaxial results obtained from the 19% Oeq material under creep, relaxation and at a constant strain rate of 8.10^{-7} s^{-1} tests have shown a different behaviour than those obtained for the 14% Oeq material, Figure 5. The strains measured from the long period creep tests continued significantly beyond the locus of the relaxed tests at all of the stress levels tested. Also, the deformation curve obtain at 8.10^{-7} s^{-1} exhibited significantly higher stresses than those obtained from the relaxation tests. These results indicate that the material equilibrium curve required by some unified models is not always path independent.

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References


Figure 1: Uniaxial constant strain rate test results and simulations

Figure 2: Experiment and simulation of CT specimens load vs. displacement
Input from FE programme

$\varepsilon_i, \sigma_i, \Delta \varepsilon_i, \Delta t$

Initialise new strains:

$\varepsilon_i = \varepsilon_i + \Delta \varepsilon_i$

(eqns. 4-7)

$\varepsilon_{eq}, \sigma_{eq}, \Delta \varepsilon_{eq}, \varepsilon_{eq}$

(eqns 8-9)

$\dot{\varepsilon}_{eq}, \frac{\partial \dot{\varepsilon}_{eq}}{\partial \varepsilon}, \frac{\partial \dot{\varepsilon}_{eq}}{\partial \sigma}$

(eqn. 12)

$\Delta \varepsilon_{eq}^{el} = f(\Delta \varepsilon_{eq}^{total}, \dot{\varepsilon}_{eq}^{in}, \frac{\partial \dot{\varepsilon}_{eq}^{in}}{\partial \varepsilon}, \frac{\partial \dot{\varepsilon}_{eq}^{in}}{\partial \sigma}, \Delta t, \theta)$

$\Delta \varepsilon_{eq}^{inelastic} = \Delta \varepsilon_{eq}^{total} - \Delta \varepsilon_{eq}^{elastic}$

(Total deformation relationship, eqn. 13)

$\Delta \varepsilon_i^{inelastic} = f(\Delta \varepsilon_{eq}^{inelastic}, \sigma_{eq}, \sigma_i)$

$\Delta \varepsilon_i^{elastic} = \Delta \varepsilon_i^{total} - \Delta \varepsilon_i^{inelastic}$

(Hooke’s law)

$\Delta \sigma_i = f(\Delta \varepsilon_i^{elastic})$

$\sigma_i^{t+1} = \sigma_i^t + \Delta \sigma_i$

Return to FE programme

Figure 3: Material solution procedure
Figure 4: FE simulations of CT specimens using plane stress or plane strain conditions and two load point displacement rates

Figure 5: Uniaxial creep, relaxation and constant strain rate tests at room temperature of 19% Oeq CP titanium