Investigation on ductile fracture of an aluminium alloy using a mean-field crystal plasticity framework

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Abstract. The onset of ductile fracture can be described by a simple damage parameter, which accounts for the accumulation of damage under arbitrary deformation. The damage parameter is usually given as integral form of strain over loading history which also has been described as a function of stress state. While the evolution of strain field can be experimentally determined using digital image correlation, experimental measurement of the multiaxial stress state is still a challenging task. Therefore, various uncoupled fracture criteria rely on stress states calculated from phenomenological plasticity model. As a result, the number of mechanical tests required to calibrate the fracture criterion may significantly increase when an anisotropic constitutive model is used. We propose an alternative approach on the basis of a mean field crystal plasticity (VPSC) model, which accounts for the microstructural features such as slip system, crystallographic texture and its evolution. While stress fields can be obtained from the use of full-field crystal plasticity framework, the proposed method utilizes the mean field crystal plasticity framework and repeat the stress estimation on various spatially resolved locations to which DIC technique provides strain history. The repeated VPSC calculations at various locations efficiently provide the map of stress evolution. The resulting map of spatially resolved stress response is further validated by comparing with the bulge stress strain curves.

1. Introduction
Uncoupled fracture criteria introduce a damage indicator which indicates the onset of fracture by a scalar function of stress and strain history [1]. Doing so, it requires the constitutive behaviour of material that is calculated by phenomenological plasticity model [2]. The material parameters associated with strain evolution can be easily obtained by the digital image correlation (DIC). However, it is still difficult to accurately measure multiaxial flow stresses. Therefore, the stress and other stress-associated quantities such as triaxiality and Lode angle usually rely on the calculation by a chosen phenomenological plasticity model. In conventional phenomenological plasticity theory, the material anisotropy is regarded constant during the plastic deformation, and this assumption may not be appropriate because a large amount of plastic strain occurs for ductile materials until fracture. In this study, a preliminary study is conducted to investigate the possibility to use a mean-field self-consistent crystal plasticity model instead of the phenomenological plasticity model to estimate stress states. A simple and direct method to utilize the field strain data from DIC for a mean-field crystal plasticity is introduced.
2. Method

2.1. Models
The mean-field crystal plasticity framework of Visco-Plastic Self-Consistent (VPSC) model [3] was utilized in this study. In it, a power-law relationship between the local strain rate $\dot{\varepsilon}$ and local stress $\sigma$ is assumed:

$$\dot{\varepsilon} = \dot{\gamma}_0 \sum_s m^s \left(\frac{m^s \cdot \sigma}{\tau_c^s}\right)^n$$

Eq. 1

where $\dot{\gamma}_0$, $m^s$ and $\tau_c^s$ denote the reference shear strain rate, Schmid tensor and the critical resolved shear stress (CRSS), respectively. The exponent $n$ is related to strain rate sensitivity and fixed as 20 in this study. The Schmid tensor $m^s$ were constructed by assuming that $\{111\} <110>$ slip systems are available for a chosen aluminium alloy AA6061-T6 sample. The CRSS $\tau_c^s$ may evolve using a Voce-hardening law:

$$\tau_c^s = \tau_0^s + (\tau_1^s + \theta_1^s \Gamma) \left(1 - \exp\left(-\Gamma \frac{\theta_0^s}{\tau_1^s}\right)\right)$$

Eq. 2

in which the symbol $\Gamma$ denotes the accumulated shear strain; The symbols $\tau_0^s$, $\tau_1^s$, $\theta_0^s$ and $\theta_1^s$ are the strain hardening behaviour. The equivalent inclusion method [4,5] for visco-plastic inclusion embedded in the visco-plastic medium [3,6] leads to the visco-plastic macroscopic constitutive description:

$$\ddot{\epsilon}_{ij}^{vp} = \bar{M}_{ijkl}^{vp} \dddot{\varepsilon}_{kl}^{vp} + \dddot{\varepsilon}_{ij}^{vp}$$

Eq. 3

where $\dddot{\varepsilon}^{vp}$ and $\bar{M}_{ijkl}^{vp}$ are the macroscopic stress and strain tensor, respectively; and $\dddot{\varepsilon}_{ij}^{vp}$ and $\dddot{\varepsilon}_{ij}^{vp}$ are the macroscopic visco-plastic compliance and back-extrapolated term, respectively. The macroscopic quantities (i.e., $\bar{M}_{ijkl}^{vp}$ and $\dddot{\varepsilon}_{ij}^{vp}$) are functions of micromechanical properties, which are a priori unknowns and are iteratively determined.

2.2. Experiments
Experimental data obtained from X-ray diffraction, bulge tests, uniaxial tension tests, and Nakajima tests were conducted. X-ray diffraction was performed using a Bruker D8 Discovery machine with a Co Kα target. The crystallographic orientation distribution was obtained from experimental pole figures using MTEX, from which a population of 6000 discrete orientations was extracted. The reconstructed pole figures from the orientation population are shown in Figure 1. Bulge test was performed using an Erichsen bulge tester model 161 on specimens with a dimension of $300 \times 300 \text{mm}^2$. Hydraulic pressure and dome height together with the images obtained from 3D stereo camera system were used to obtain the flow stress-strain curve. Uniaxial tension tests along rolling, diagonal, and transverse directions were performed according to the ASTM E8 standard. Strain rate was about $4.3 \times 10^{-4} \text{s}^{-1}$.

A Nakajima test was conducted following the ISO standard 12004-2. The diameter of punch was 100 mm, and the stroke speed was fixed as 0.5 mm/s. Square specimens were tested to induce a near balanced biaxial state. DIC analysis was applied to obtain strain fields that develop on the top surface of specimens subjected to the Nakajima test. The evolution of deformation gradient tensor $F$ with respect to test time was collected at a set of spatial coordinates of interest near fracture site.

2.3. VPSC simulation condition
The polycrystal aggregate used in VPSC calculation was characterized by the discrete orientations and the Voce hardening parameters calibrated by fitting with the flow stress-strain curve resulting from the bulge test. The tangent linearization method was assumed in the current study. The goodness of the VPSC fit is well illustrated in Figure 2. The calibrated parameters are given in Table 1.
The VPSC simulation was conducted to estimate the stress fields corresponding to a set of spatial locations at which the digital images were collected during the Nakajima tests. As the deformation obtained from DIC includes both strain and spin, the deformation gradient tensor is required to fully reflect the behaviour of each spatial point. However, as the DIC was applied to the top surface of specimen, only $F_{11}, F_{12}, F_{21}$ and $F_{22}$ components can be experimentally obtained. The other components associated with the thickness direction (namely $F_{13}, F_{23}, F_{31}, F_{23}$ and $F_{33}$) cannot be experimentally determined. To that end, the assumption of incompressibility and zero thickness-related shear components were applied. The determinant of $F$ is related to the volume change:

$$\frac{dv}{dV} = \det(F)$$

Eq. 4

where $dv$ and $dV$ denote the volume elements before and after the deformation, respectively. The incompressibility condition (i.e., $dv = dV$) leads to $\det(F) = 1$. Additionally, by assuming $F_{13} = F_{31} = F_{23} = F_{32} = 0$, the determinant is expressed as:

$$\det(F) = F_{11}F_{22}F_{33} - F_{12}F_{21}F_{33} = F_{33}(F_{11}F_{22} - F_{12}F_{21}).$$

Eq. 5

As a result of this assumption, the thickness component of deformation gradient can be estimated as $F_{33} = 1/(F_{11}F_{22} - F_{12}F_{21})$.

The deformation gradient tensor may contain a significant amount of experimental noise. Savitzky-Golay filter [7] as implemented in SciPy package [8] was applied in order to reduce the noise in the experimental data. A series of discrete $F_{ij}$ values corresponding to a batch of sequential images are fitted to a polynomial function of a chosen order. The smoothed $F$ tensor is used to determine the boundary condition, to which the VPSC polycrystal aggregate is subjected. In a recent study, it was shown that although the degree of smoothing is affected by the choice of the order of polynomial and the size of batch used in the Savitzky-Golay filter, the VPSC-calculated stress is not significantly affected [9]. The smoothed deformation gradient is multiplicatively decomposed to stretch $U$ and rotation $R$ tensors such that:

$$F = R \cdot U$$

Eq. 6

From the stretch tensor, the engineering strain $\varepsilon$ is obtained as:

$$\varepsilon_{ij} = U_{ij} - \delta_{ij},$$

Eq. 7

where $\delta_{ij}$ is the Kronecker delta. The logarithmic strain $\varepsilon$ is:

$$\varepsilon_{ij} = \delta_{ij} \ln(1 + \varepsilon_{ij}) + (1 - \delta_{ij})\varepsilon_{ij}.$$  

The rate of rotation $\dot{R}$ can be estimated using the Euler method:

$$\dot{R}_{ij}^{(n+1)} = \frac{R_{ij}^{(n+1)} - R_{ij}^{(n)}}{\tau^{(n+1)} - \tau^{(n)}}$$

Eq. 8

in which the superscripts $(n + 1)$ and $(n)$ denote the time steps at which the relevant digital images were acquired. The same was applied to obtain the logarithmic strain rate $\dot{\varepsilon}$. Both rates of rotation and strain were directly employed to VPSC at the various spatial locations selected on the top surface of specimen deformed by the Nakajima test.
Figure 1 (111), (200), and (220) pole figures reconstructed from the population of 6000 discrete orientations

Figure 2 Experimental flow stress-strain curves from bulge test and the VPSC model fit

|       | $\tau_0$ | $\tau_1$ | $\theta_0$ | $\theta_1$ |
|-------|----------|----------|-------------|------------|
|       | 92.72    | 58.85    | 391.6       | 11.26      |

Table 1 Voce hardening parameters
Figure 3 Experimental true stress-strain curves and model predictions

Figure 4 Strain map obtained from the DIC at the final step prior to the onset of fracture
Figure 5 Nominal components of strain and stress corresponding to the digital image just prior to fracture.
Figure 6 Nominal components of strain and stress corresponding to the equivalent strain of 0.4
Figure 7 Major and minor principal strain obtained by DIC on spatially resolved points, from which VPSC inputs were obtained.

Figure 8 Major and minor principal stresses calculated by VPSC.

Figure 9 Triaxiality calculated by VPSC.
3. Results and discussion

The VPSC model with the parameters calibrated by the bulge test systematically underestimated the uniaxial tension flow stress responses as shown in Figure 3. Nevertheless, the isotropic response regardless of direction was captured by the VPSC model. Figure 4 shows the entire strain map resulting from the DIC analysis using the images obtained during the Nakajima test. The VPSC simulation was conducted for a more confined region near the fracture. To that end, a grid consisting of 163 locations that are equally distanced within a 46 mm × 40 mm area was selected near the fracture site. The strain components obtained from DIC analysis corresponding to this selected area are shown in terms of $\varepsilon_{11}$, $\varepsilon_{12}$, and $\varepsilon_{22}$ in the left column of Figure 5. It should be noted that the coordinate origin ($X = 0, Y = 0$) in Figure 5 corresponds to the coordinate ($X = 64, Y = 52$) in Figure 4. The same applies to $X$, $Y$ coordinates in Figures 5-9 as well. The stress resulting from VPSC calculation for the chosen grid is shown on the right column of Figure 5-6. The major and minor components of principal strain and stress are shown in Figures 7 and 8, respectively.

Figure 5 shows that the normal stress components $\sigma_{11}$ and $\sigma_{22}$ near the fracture amounts to 400–500 MPa. The corresponding normal strain components $\varepsilon_{11}$ and $\varepsilon_{22}$ shown in Figure 5 are around 0.25–0.30, which correspond to an equivalent strain of 0.5–0.6 for the case of bulge test. The maximum strain available obtained from the bulge test was limited to 0.4 as shown in Figure 2, so that a direct comparison between the bulge and the VPSC-calculated result at fracture is not plausible. Nevertheless, Figure 6 indicates that the VPSC-calculated stress at the equivalent strain of 0.4 amounts to 420–460 MPa, which is marginally different from the corresponding stress from bulge test (i.e., 410 MPa). This suggests that the stress estimated by VPSC at fracture should not be significantly different from the actual stress state. Figures 7-8 show the map of principal strains and the corresponding VPSC-calculated principal stresses. Although the VPSC-predicted principal stresses are a bit noisy, the region of the maximum stress well corresponds to the one with maximum principal strain shown in Figure 7. Figure 9 shows that the stress triaxiality predicted by VPSC amounts to around 0.66, which is reasonable considering that the circular specimen was used in the Nakajima test to induce balanced biaxial stress state. The stress states and the triaxiality calculated by VPSC model through the direct employment of DIC raw data after smoothing by Golay-Savitzky method seem quite reasonable. Therefore, it is expected that an alternative uncoupled ductile fracture criterion can be suggested by repeatedly conducting the mean-field VPSC calculations for various locations near fracture. An advantage of using the mean-field VPSC model over the use of full-field crystal plasticity is the efficiency of calculation: the total running time of VPSC was about 4 minutes for the entire spatial locations shown in Figure 5-9 using a work station with 48 CPU core units.

4. Conclusions

In this study, a mean-field self-consistent crystal plasticity model has been applied to investigate its applicability for ductile fracture criterion, which requires the evolution of stress states corresponding to arbitrary strain history. A Visco-Plastic Self-Consistent polycrystalline aggregate was calibrated for an aluminium AA6061-T6 sample by bulge test and X-ray diffraction, which shows a reasonable predictive accuracy on uniaxial tension flow stress-strain curves. The stresses calculated by VPSC at various locations near fracture seem reasonable in comparison with the bulge test result. Also, the triaxiality map estimated by the VPSC-predicted stress seems reasonable for a near balanced biaxial state realized through a Nakajima test. Therefore, it is expected that the method introduced in this study can provide an efficient alternative plasticity model for an uncoupled ductile fracture criterion, in which both strain and stress states are required. As a follow-up study, further investigation to develop a fracture criterion applicable for a wider range of stress and strain states is required.

5. References

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