A framework of modelling slip-controlled crack growth in polycrystals using crystal plasticity and XFEM

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Abstract. Short cracks tend to develop at high and irregular rates compared to macroscopic cracks, making the prediction of fatigue life a challenging task. In this work, a numerical framework combining crystal plasticity model and the Extended Finite Element Method (XFEM) is applied to study the slip-controlled short crack growth in a polycrystal superalloy RR1000. The model is calibrated from experiments and used to evaluate short crack growth paths and rates. Two fracture criteria are used and compared: the onset of fracture is controlled by the total and individual cumulative shear strain respectively, and the crack grows either perpendicular to the direction of maximum principal strain or along crystallographic directions.

1. Introduction
Numerous experiments have observed that early-stage cracks exhibit a propagation behaviour different from long cracks, having tortuous slip-controlled crack path and fluctuations in crack growth rate, and being highly affected by the local microstructure.

To numerically study short cracks, various techniques have been adopted to simulate the initiation and propagation. The recently proposed Extended Finite Element Method (XFEM) (Moës et al., 1999) introduces enrichment functions into the standard FEM to describe arbitrary discontinuous structures, thus allows us to model cracks in a mesh-independent way, without predefined paths or remeshing.

Meanwhile, a number of microscopic fracture criteria have been developed to simulate short crack growth in metals. Specifically, crystal plasticity (CP) theory is embedded to introduce crystallographic mechanism, which allows us to capture the behaviour of early-stage cracks. For example, the total cumulative plastic strain was employed to evaluate the crack growth (Zhao and Tong, 2008) and further used to recover the crack path in a polycrystalline Ni-based superalloy (Lin et al., 2011). The
slip trace corresponding to the maximum cumulative slip was set as the crack path without considering the intragranular deflection of crack growth. In other studies, XFEM and CP were combined to investigate the crack growth in single crystals (Zhang et al., 2020) and polycrystals (Wilson et al., 2019). This approach can capture the alternating crack path and the variations in propagation rate, but more work is still required to improve this method for a better understanding of the short crack behaviour.

In this study, we aim to develop a framework that combines the CP and XFEM to model the short crack propagation in polycrystals. The CP model was calibrated against the experimental data of RR1000 material and applied to an artificial polycrystal model. The individual cumulative shear strain proposed in our previous study (Zhang et al., 2020) was adopted to reflect the contribution of crystallographic mechanism. Two different crack growth criteria were examined and compared. Finally, orientations of the polycrystal were changed to show the randomness of early-stage cracks.

2. Methodology

2.1. Crystal plasticity (CP) model

The crystal plasticity model used here is based on the slip-based and rate-dependent classical CP theory (Peirce et al., 1982), in which the plastic shear rate of each slip system takes the form

$$\dot{\gamma}^\alpha = \dot{\gamma}_0 \left( \frac{\tau^\alpha}{\tau_0} \right)^n \text{sign}(\tau^\alpha).$$

(1)

The isotropic hardening is built upon the evolution of the critical shear stress as follows

$$g^{(\alpha)}(\dot{\gamma}^{(\beta)}) = \sum_{\beta} h_{\alpha\beta} \dot{\gamma}^{(\beta)},$$  

$$h_{\alpha\beta} = q_{\alpha\beta} h_{\beta}$$

$$h_{\beta} = h_0 \text{sech}^2 \left( \frac{h_0 \gamma}{\tau_s - \tau_0} \right).$$

(2)

and total cumulative shear strain on all slip systems is obtained as

$$\gamma = \sum_{\alpha} \int_0^t \dot{\gamma}^\alpha dt.$$  

(3)

For detailed explanations of CP theory and equations, please refer to our previous work (Zhang et al., 2020). The CP model described above was implemented in ABAQUS/Standard finite element software as a user material subroutine (UMAT).

2.2. XFEM strategies

XFEM implemented in ABAQUS was used in this study and a user damage subroutine (UDMGINI) was used to control the development of cracks, where the damage indicator value and the vector normal to the crack growth direction are provided. During each computation increment, the onset of fracture is determined by the fracture value and a normal direction vector averaged at the centroid of an element. When the fracture value is greater than 1.0, the traction-separation behaviour is activated and the crack grows along the given direction.

To investigate the crack growth behaviour, two different damage criteria were used and compared in this work. For the first one, the crack will propagate when the total cumulative shear strain at the crack tip is larger than the set value (1.5E-2), and the crack path is perpendicular to the direction of the maximum principal strain. We use MP (maximum principal strain) to represent this criterion. In the crystallographic criterion, the crack will initiate when the highest individual cumulative shear strain of all slip systems at the crack tip exceeds the limit (1.0E-2), then the crack will grow along the corresponding slip plane. We use SP (slip plane) to indicate this criterion. The limits chose here were arbitrary since they have been proved to have little influence on the crack path (Zhang et al., 2020).
3. Numerical modelling

To simulate the crack propagation in polycrystals, this work focused on the polycrystalline alloy RR1000. It has a fine grain structure (average grain size of 4.76 μm) and random crystallographic orientation.

3.1. CP calibration

In the calibration of CP model, a plane-strain representative volume element (RVE) was used to produce the overall mechanical response under cyclic loading (shown in Fig. 1a). The artificial grain microstructure was generated by employing the Voronoi tessellation algorithm. According to previous studies (Lin et al., 2011), the RVE can produce a converged response when the RVE contains at least 150 grains and 4000 elements, which was adopted in this work.

![Fig. 1 (a) The geometry of RVE used in the CP calibration; (b) comparison of the first hysteresis loop of numerical results and experimental data.](image)

Table 1. Parameters of the CP model

| Parameters | \(C_{11}/\text{MPa}\) | \(C_{12}/\text{MPa}\) | \(C_{44}/\text{MPa}\) | \(n\) | \(\dot{\gamma}_{c}/\text{sec}^{-1}\) | \(h_{0}/\text{MPa}\) | \(\tau_{s}/\text{MPa}\) | \(\tau_{0}/\text{MPa}\) | \(q_{\text{max}}\) | \(q_{\text{off}}\) |
|------------|-----------------|-----------------|-----------------|-----|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|
|            | 166200          | 66300           | 100100          | 10  | 0.00001         | 160.0           | 251.0           | 230.2           | 1               | 1               |

3.2. Crack propagation model

In the crack propagation model, the same 2D model was adopted but under different cyclic loading (loading ratio R=0.1). A denser mesh was used to capture the short crack behaviour better, thus 11608 quadrilateral linear plane strain (CPE4) XFEM elements with an average size of ~0.6 μm were created, which has been proved by Zhang et al. (2020) to produce converged results. A pre-defined crack of 0.015mm was also introduced to the top of the model to initiate the crack propagation.
Fig. 2 The model and boundary conditions used for the crack growth simulation.

4. Results and discussion

4.1. Deformation around the crack tip

Before the first crack growth, the deformation distribution around the crack was extracted. In Fig. 3a, the distribution of strain along the loading axis varies in different grains, showing the diversity of crystal property. Due to the orientation difference, grains will have ‘hard’ or ‘soft’ responses and affect how the crack grows. Similar trends can be observed in the distribution of total cumulative shear strain (Fig. 3b), but with a clearer area right ahead of the crack tip. Since the distribution of total cumulative shear strain is plastic deformation, it shows that slip behaviour is more active at two sides of the crack tip.

4.2. Crack growth path

The 2D model was subjected to cyclic loadings and cracks were predicted according to the MP (Maximum principal strain) and SP (Slip plane) criterion. Crack paths of each case as well as distributions of the cumulative shear strain were depicted in Fig. 4. MP model 1 and SP model 1 used the same crystal orientations, and a new set of orientations were specified to SP model 2 to examine the effect of crystal orientations.

It is observed that the predicted crack in MP model exhibited Mode-I behaviour (Fig. 4a), being vertical to the loading axis. The crack went through several grains along slightly different directions. On the contrary, cracks predicted by SP models show different trends (Fig. 4b and c), being similar to experimental observations. Transgranular cracks grew along favourable slip planes in each grain.
showing tortuous crack paths. Multiple deflections were noticed at both grain boundaries and grain inside, which is due to the alternation of dominating slip systems.

![Cracks predicted by MP and SP models as well as distributions of cumulative shear strain.](image)

Looking at the distribution of cumulative shear strain, we noticed that the crack in MP model developed out of the intensely deformed domain while cracks in SP models grew around the high-value area, which will cause high fluctuations in their propagation rates. For instance, when the crack of SP model 1 grew into the high ICSS area, the crack can easily go through the whole grain since the area ahead of the crack tip had already reached the fracture limit.

Comparing the results of SP model 1 and 2, it is noticed that generated cracks developed along totally different paths. Though the change of orientations will not affect the macroscopic response, it altered the distribution of ‘hard’ and ‘soft’ grains and also the dominating slip systems.

### 4.3. Comparison of crack growth rates

Meanwhile, the crack growth speeds were measured and grouped in Fig. 5. Here the crack paths were projected to the normal direction of the loading axis since the propagation paths were not horizontal.

![Comparison of crack growth rates.](image)

It is noted that all curves exhibit a step change of shape with increasing loading cycles as a result of random crystal orientations. Different slip activities in each grain can speed up or slow down the current propagation rate. On the other hand, it is noticed that more steps can be found in SP models, not only when cracks went through boundaries but also propagated inside grains, which is attributed to
the intragranular path change (see outlined A and B in Fig. 5). Besides, changing orientations can cause huge differences to crack growth rates, although it has little influence on the global mechanical response.

5. Conclusions
A numerical framework using crystal plasticity and XFEM was employed in this study to evaluate the short crack propagation in RR1000 polycrystal. The framework can predict transgranular short crack path at an acceptable computing expense, and both macroscopic and microscopic damage criteria were examined and compared. Results show that the crystallographic damage criterion can better recover the experimentally observed short crack growth behaviour. In conclusion, this research contributes to the understanding of short crack propagation and allows for further modifications.

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