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Realistic microstructure-based modelling of cyclic deformation and crack growth using crystal plasticity

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ABSTRACT

Using crystal plasticity, finite element analyses were carried out to model cyclic deformation for a low solvus high refractory (LSHR) nickel superalloy at elevated temperature. The analyses were implemented using a representative volume element (RVE), consisting of realistic microstructure obtained from SEM images of the material. Monotonic, stress-relaxation and cyclic test data at 725 °C were used to determine the model parameters from a fitting process and their sensitivity to RVE size and random grain orientation. In combination with extended finite element method (XFEM), the crystal plasticity model was further applied to predict surface crack growth, for which accumulated plastic strain was used as a fracture criterion. Again, realistic microstructure, taken from the cracking site on the surface of a plain fatigue specimen, was used to create the finite element model for crack growth analyses. The prediction was conducted for a pseudo-3D geometrical model, resembling the plane stress condition at specimen surface. The loading level at the cracking site was determined from a viscoplasticity finite element analysis of the fatigue specimen. The proposed model is capable of predicting the variation in growth rate in grains with different orientations.

1. Introduction

Polycrystalline metals and alloys possess a heterogeneous nature of grain microstructure and exhibit anisotropic response during mechanical deformation. These crystallographic orientation effects cannot be captured by traditional isotropic homogeneous models. Therefore, physically-based crystal plasticity models were developed and have been successfully applied in literature to predict the anisotropic mechanical response of individual grains in polycrystalline materials. Combination of crystal plasticity and finite element method has the ability to model the global and local stress–strain response of crystalline materials under various types of loading regimes including fatigue [1–3].

In the efforts to consider the effects of the material's microstructure on the mechanical behaviour of nickel based superalloy, a large number of studies were conducted using crystal plasticity [4–6]. These studies aimed to predict the global and local stress–strain response as well as grain texture evolution and micro-structural crack nucleation under various loading conditions. For example, Fedelich [7] employed a crystal plasticity model with implicit dependency on precipitate size and volume fraction to predict the influence of microstructural parameters such as lattice misfit on deformation behaviour of a single crystal nickel based superalloy. The model was also used to calculate the back stress as a function of local deformation state, i.e., distribution of plastic strain in the microstructure. Kumar et al. [8] adopted crystal plasticity-based finite element approach to study the effects of microstructural variability on cyclic deformation of a single crystal nickel base superalloy. This study considered the effect of size and volume fraction of the γ' precipitates on fatigue resistance of the material. Shoney et al. [9] presented a microstructure sensitive crystal plasticity model which has the capability to capture the variation in stress–strain response with changes in grain size, distribution of precipitate size and precipitate volume fraction as well as dislocation density for each slip system. In this regard, Lin et al. [10] used 2D crystal plasticity model to study the effect of grain microstructure on localised stress–strain distribution of a polycrystalline nickel based superalloy. The study was subsequently extended to 3D to simulate the global stress–strain response of the material under fatigue loading [11]. In addition, effects of grain microstructure on crack tip deformation and crack growth path were also explored using the crystal plasticity model. However, these models were limited to the use of artificial grain

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microstructure generated by employing the Voronoi tessellation algorithm, and cannot capture the local stress and strain behaviour precisely, an important indicator for nucleation of fatigue cracks. In order to capture the actual localised stress–strain response, 2D model based on realistic microstructure were developed by Choi et al. [12] to predict the localised stress in polycrystalline Mg alloys using crystal plasticity finite element method. Similarly, Wang et al. [13] studied grain level heterogeneous deformation in polycrystalline α-Ti material using crystal plasticity model based on 2D realistic microstructure. However, the work is limited to simulation of local deformation, without consideration of global deformation. Also to our best knowledge, there is hardly any work devoted to prediction of fatigue crack growth in polycrystalline materials using the realistic grain microstructure and crystal plasticity model.

Fatigue failure in engineering materials has been an important subject for several decades. A number of computational techniques have been developed and used in the literature to predict fatigue crack initiation and propagation, especially the finite element method (FEM) [14]. However, the major shortcoming of FEM is that the crack surfaces need to be in line with the edges of the elements, which presents a challenge for FEM in modelling the growth of discontinuities and cracks. In order to overcome this difficulty, a novel approach, called extended finite element (XFEM), has been developed recently [15]. In this technique, the crack geometry is mesh-independent and there is no need for the re-meshing to accommodate the crack as it grows. This is achieved by incorporating the enrichment functions into standard finite element approximation space [16,17]. With an appropriate fracture criterion, crack propagation can be modelled without the introduction of a predefined crack growth path, a unique feature of the XFEM technique. In fact, the method has already been widely applied to model a variety of crack problems such as crack propagation in thin-walled structures, crack branching and dynamic crack growth [18–20].

A variety of fracture criteria have been proposed in the last decades to predict crack propagation, which can be classified as either stress or strain based approach. For example, Erdogan and Sih [21] proposed the maximum principal stress criterion as the crack growth driving force. They suggested that the crack would propagate in the direction perpendicular to that of maximum principal stress when the stress value at the crack tip reached a critical value. Similarly, Moes et al. [22] used the circumferential stress criterion for crack growth. The direction of crack propagation was determined by setting the shear stress equal to zero as the circumferential stress was a principal stress in the direction of crack propagation. So, this was essentially a principal stress-based criterion. Newman [23] used a strain criterion for crack advancement and the crack started to grow when the strain immediately ahead of the crack tip reached a critical strain level. McDowell and Dunne [5] used the concept of accumulated plastic strain to reveal the fatigue crack formation in Ni-based superalloys. Using a crystal plasticity model, it was shown that the site of crack nucleation observed in experiments matched the location of maximum accumulated plastic strain obtained from simulations. Recently, accumulated plastic strain has been explored as a criterion to predict fatigue crack growth. This was based on the observation of strain accumulation, from both modelling [24–27] and experiments [28,29], near a crack tip under fatigue loading conditions. Also, such a criterion has been utilised to predict fatigue crack propagation in a Ni-based superalloy at elevated temperature using the XFEM technique [30]. With the assistance of a cyclic viscoplasticity model, the predicted crack propagation path and rate were in very good agreement with experimental data [30]. However, there is very limited work in predicting the full path and rate of crack propagation by considering the explicit grain microstructure, and this can be attempted by combining the XFEM technique, a crystal plasticity model and a suitable fracture criterion such as strain accumulation.

In this paper, crystal plasticity model, in combination with XFEM, has been applied to study cyclic deformation and fatigue crack growth in a nickel-based superalloy LSHR (Low Solvus High Refractory) at high temperature. The first objective of this research was to develop and evaluate a RVE-based finite element model with the incorporation of a realistic material microstructure. The second objective of this work was to determine the parameters of a crystal plasticity constitutive model to describe the cyclic deformation behaviour of the material by using a user-defined material subroutine (UMAT) interfaced with the finite element package ABAQUS. The model parameters were calibrated from extensive finite element analyses to fit the monotonic, stress relaxation and cyclic test data. The third objective was to predict crack growth by combining the XFEM technique and the calibrated crystal plasticity UMAT, for which accumulated plastic strain was used as the fracture criterion.

2. Crystal plasticity model

The theoretical framework used here is based on large deformation and rate-dependent crystal plasticity theory presented in [8,31,32]. In the theory, shear flow along slip systems is solely responsible for the plastic deformation in the crystals. The shear deformation along slip planes is caused dislocation generation and motion, with the associated inelastic velocity gradient ($\boldsymbol{L}^{\mathrm{P}}$) given as:

$$\boldsymbol{L}^{\mathrm{P}} = \dot{\boldsymbol{F}}^{\mathrm{P}}\boldsymbol{F}^{\mathrm{P}^{-1}} = \sum_{\alpha=1}^{n}\dot{\gamma}^{\alpha}(\mathbf{s}^{\alpha}\otimes\mathbf{m}^{\alpha}) \tag{1}$$

where $\boldsymbol{F}^{\mathrm{P}}$ is plastic deformation gradient, $\dot{\gamma}$ is shear strain rate of slip system α, and unit vectors $\mathbf{s}^{\alpha}$ and $\mathbf{m}^{\alpha}$ refer to the direction of shear slip and the normal to the slip plane, respectively.

The shear strain rate ($\dot{\gamma}^{\alpha}$) for each slip system can be expressed in terms of the resolved shear stress (τ^{α}) using an exponential function:

$$\dot{\gamma}^{\alpha} = \dot{\gamma}_0 \exp\left[\frac{-F_0}{\kappa\theta}\left\langle 1 - \left\langle \frac{|\tau^{\alpha} - B^{\alpha}| - S^{\alpha}\mu/\mu_0}{\hat{\tau}_0\mu/\mu_0}\right\rangle^{p}\right\rangle^{q}\right]\mathrm{sgn}(\tau^{\alpha} - B^{\alpha}) \tag{2}$$

where S^{α} is the slip resistance, B^{α} is the back stress, μ and μ_0 are shear moduli at absolute temperature and 0 K, respectively, and κ is the Boltzmann constant. In Eq. (2), F_0, $\hat{\tau}_0$, p, q and $\dot{\gamma}_0$ are material constants which need to be calibrated for proper simulation of the material behaviour.

The slip resistance and the back stress are two internal state variables which are associated with the current dislocation network introduced at the slip level. Specifically, the slip system resistance (S^{α}) is a measure of the impedance of dislocation motion on a slip system by short-range interactions between all dislocations [33]. The slip resistance for a slip system can be described by the following equation:

$$\dot{S}^{\alpha} = \left[h_s - d_D(S^{\alpha} - S_0^{\alpha})\right]|\dot{\gamma}^{\alpha}| \tag{3}$$

where S_0^{α} is considered as initial value of the slip resistance for a slip system, and h_s and d_D are the material constants linked to static and dynamic recovery terms, respectively.

The back stress is associated with dislocations bowing between obstacles, such as precipitates or pinning points, and can be expressed in terms of a hardening constant (h_B) and a dynamic recovery constant (r_D), as:

$$\dot{B}^{\alpha} = h_B\dot{\gamma}^{\alpha} - r_D B^{\alpha}|\dot{\gamma}^{\alpha}| \tag{4}$$