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Material characterisation and finite element modelling of cyclic plasticity behaviour for 304 stainless steel using a crystal plasticity model

Jiawa Lu*, Wei Sun, Adib Becker

Department of Mechanical, Materials and Manufacture Engineering, The University of Nottingham, University Park, Nottingham NG7 2RD, UK

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ABSTRACT

Low cycle fatigue tests were carried out for a 304 stainless steel at room temperature. A series of experimental characterisations, including SEM, TEM, and XRD were conducted for the 304 stainless steel to facilitate the understanding of the mechanical responses and microstructural behaviour of the material under cyclic loading including nanostructure, crystal structure and the fractured surface. The crystal plasticity finite element method (CPFEM) is a powerful tool for studying the microstructure influence on the cyclic plasticity behaviour. This method was incorporated into the commercially available software ABAQUS by coding a UMAT user subroutine. Based on the results of fatigue tests and material characterisation, the full set of material constants for the crystal plasticity model was determined. The CPFEM framework used in this paper can be used to predict the crack initiation sites based on the local accumulated plastic deformation and local plastic dissipation energy criterion, but with limitation in predicting the crack initiation caused by precipitates.

1. Introduction

304 stainless steel is a type of austenitic steel widely used in pipes of chemical plants and many other applications which may be subject to cyclic loading conditions. The predictions of fatigue life and crack initiation sites are important aspects of designing the plant structure. Fatigue failure is usually caused by the creation of microcracks smaller than the grain size, then the growth and coalescence of micro flaws to a dominant crack, followed by stable propagation of the dominant macrocrack, and structural instability or complete fracture finally.

Microcrack nucleation is influenced by a range of mechanical, microstructural and environmental factors. Dunne [1] investigated the microcrack initiation and propagation for FCC nickel-based super-alloy phenomenon. It was found by experimental observation that fatigue induced microcracks smaller than the grain size could initiate at multiple locations, including grain boundaries, precipitates, PSBs, and surface inclusions and extrusions. These microcracks grow by coalescence to form a dominant crack, which is influenced strongly by the grain orientation. In addition, not all microcracks would propagate, and the slip propagation direction is parallel with the active slip direction within the grain. It was further pointed out by Bhat [2] that the crack initiation sites depend on the applied loading. For high cycle fatigue when the strain amplitude is low, strain tends to be localised at persistent slip bands and this is where the crack initiates. On the contrary, for low cycle fatigue when the strain amplitude is high, the grain boundary becomes the crack initiation site, since dislocations pile up at the grain boundary. For the intermediate strain amplitude, damage initiates on both grain boundary and slip traces. It is also concluded by Hanlon [3,4] that fatigue crack initiation sites depend on the grain size and grain size arrangement. Crack initiation is favoured in a coarse-grain material compared to a fine grain material. Grain refinement increases the fatigue limit, while reducing the microcrack initiation threshold, but it also increases the fatigue crack growth rate. Based on a study on waspaloy [5,6], it was also pointed out that the crack initiation sites tend to be larger than the average grain size, but not necessarily the largest grain size. The crack initiation grains normally are located within some cluster of grains with misorientations less than 15°, which act similar to a large single grain.

The crystal plasticity method is a systematic method which relates the micro-scale material properties, relating to grain and morphology, to the mesoscale mechanical behaviour. The pioneering work of the crystal plasticity method was performed by Taylor [7] for face cubic centred (FCC) polycrystals subject to large plastic strains, in which it was assumed that the strain in each grain was homogeneous and equal to the macroscopic

* Corresponding author.
E-mail address: eaxjl2@nottingham.ac.uk (J. Lu).

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Nomenclature

$\boldsymbol{L}$	Velocity gradient
$\boldsymbol{F}$	Deformation gradient
$\boldsymbol{\sigma}$	Stress
$\boldsymbol{\varepsilon}$	Strain
$\boldsymbol{m}$	Slip direction
$\boldsymbol{n}$	Slip normal
D	Deformation tensor
$\boldsymbol{R}$	Rotation matrix
$\boldsymbol{\omega}$	Lattice spin tensor
$\boldsymbol{A}$	Dislocation interaction matrix
V	Volume
G	Shear Modulus
b	Burger's vector
Δ	Range
*	Lattice deformation
p	Plastic deformation
$\boldsymbol{\Omega}$	Rotational tensor
2θ	Bragg angle
Cij	2nd order elastic moduli matrix
$\mathcal{L}_{ijkl}$	4th order elastic moduli tensor
γ	Shear strain
τ	Shear stress
g	Critical shear stress
χ	Backstress
ρ	Dislocation density
α, β	Index of slip system
$\boldsymbol{\mu}$	Schmid factor
y_c	Critical annihilation length

polycrystalline strain. In addition, it was proposed that at least five slip systems should be available for the plastic deformation, and the minimum work principle was used to determine the five active slip systems. This model is quite limited in application since this transition model linking the local to the bulk material behaviour did not consider the grain interactions. However, when the crystal plasticity method is employed in the finite element (FE) method, the stress equilibrium and strain compatibility are automatically achieved by the built-in ability of the FE solver for modelling polycrystals. With the introduction of the dislocation dynamics simulations by Devincre and Kubin [8,9], the crystal plasticity method has been backed with a solid physical-based understanding from the elementary dislocation mechanism.

Since microcrack initiation smaller than the grain size highly depends on the grain arrangement, the prediction of microcrack initiation is normally based on the crystal plasticity framework. Fine and Bhat [10] proposed an energy approach to estimate the number of cycles to initiate microcracks in single crystal iron and copper, by balancing the energy required to form the crack surfaces and the energy released from storage. Voothaluru and Liu [11] applied the energy method into the crystal plasticity framework to predict crack initiation life for the randomly generated grain microstructures of a polycrystalline copper, and to identify the potential weak sites in fatigue behaviour. Tanaka and Mura [12] proposed a crack nucleation life rule based on the assumption that microcracks were initiated by irreversible dislocation pile-ups in PSB. Several works [13,14] modelled the prediction of the crack initiation in polycrystalline steel based on Mura's rule, as well as investigated the relationship between crack densities, crack imitation rate and cycle number. In addition to the above method, there are a variety of crack initiation indicators developed to predict microcrack initiation sites and to determine the number of cycles leading to microcrack initiation, such as the accumulated plastic deformation $p = \int_0^T (\frac{2}{3}\boldsymbol{L^p}:\boldsymbol{L^p})^{\frac{1}{2}}dt$ in Manonukl and Dunne [15] and local plastic dissipation energy $E_p = \int \boldsymbol{\sigma}:\boldsymbol{L_p}dt$ in Cheong et al. [16] . Therefore, it is important to understand the local stress and strain distribution based on a given grain orientation and grain arrangement. The crystal plasticity method, which predicts the macroscopic plastic behaviour by examining the microscopic anisotropic crystal behaviour, is a powerful tool to study the microstructure influence on the fatigue failure. The microscopic factors usually involve slip with the associated dislocation, texture and grain shape, in the context of continuum mechanics. However, it is also argued [17] whether these crack initiation indicators would lead to a fatal flaw. By comparing the crack initiation experimental results by DIC and FE simulation results by crystal plasticity, Cheong et al. [16] also pointed out that high energy sites are not necessarily the crack initiation sites; however, crack initiation sites must have high energy.

There are several studies which deal with austenitic steels including stainless steel 304L and 316L using CPFEM. Le Pécheur et al. [18] used the dislocation density-based model by constructing a 3D aggregate to investigate the effect of pre-hardening, which leads to a more homogeneous local stress and strain distribution at the stabilised fatigue region. In addition, a variety of damage initiation criteria were applied to aggregates of different surface roughness to investigate the sensitivity of these criteria to the roughness profile and pre-hardening. Feaugas and Pilvin [19] reviewed the dislocation pattern related to the hardening stages, and introduced the dislocation structure into the constitutive equations of a single crystal, including walls and channels. Li et al. [20,21] considered the softening effect in the stainless steel and studied the overload effect and the influence of the loading path. Schwartz et al. [22] employed a non-local approach to account for the strain gradient between adjacent points, which gives a better prediction of the tensile and fatigue tests for materials of a variety of grain sizes. Guilhem et al. [23,24] pointed out the cluster effect for the local fracture, such as grain location, grain arrangement and interaction. Sweeney et al. [25] compared the crack initiation sites observed from four-point bending test and those obtained from CPFEM simulation. Elastic anisotropy was found to be vital in the microstress and slip distributions. In addition, the locations of the peak density of geometry necessary dislocations were coincident with the peak effective plastic strain, dominant accumulated plastic slip and the experimentally observed crack initiation sites.

The aim of the current paper is to build up a framework of the CPFEM, and to investigate the crack initiation criterion based on this model. Section 2 introduces the theory of CPFEM, including the kinematics and hardening behaviour of a single crystal, as well as the transition rule between a single crystal and polycrystals. Section 3 outlines the experimental methodology relating to the model, including detailed procedure for material characterisation and the method for determining the material constants. Section 4 illustrates the CPFEM model development and the main simulation results. The experimental and modelling results are discussed and concluded in Section 5.

2. Theory

The crystal structure of the austenitic steel is FCC, which has only one set of slip system $\{111\}<110>$, and comprises a total of twelve slip systems that can take part in the plastic deformation.